Reversible 1,2-Alkyl Migration to Carbene and Ammonia Activation in an NHC-Zirconium Complex.

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Contents

1. Experimental details:

All experiments were performed using conventional vacuum line and Schlenk tube techniques or in a glovebox under nitrogen atmosphere. Solvents were dried by the method of Grubbs.[1] Complex **1** was prepared according to our previous report.[2] Benzene-d_6 and toluene-d_8 were degassed and passed through a plug of activated alumina prior to use. NMR spectra were recorded on Varian Mercury 300, Varian INOVA 500, Varian INOVA 600 or Bruker 400 spectrometers and referenced to the solvent residual peak. Elemental analyses were performed by Robertson Microlit Laboratories, Inc., Ledgewood, NJ 07852.

Synthesis of complex 2: In a Schlenk bomb, complex **1** (0.10 g, 0.125 mmol) was dissolved in 10 mL toluene and trimethylphosphine was added (26 μL, 0.250 mmol). The flask was sealed and warmed during one hour at 50 °C. Then, the solution was evaporated and the residue was dissolved in pentane. After filtration through a plug of celite and evaporation, complex **2** was obtained as light yellow powder (91 mg, 83% yield). ^{1}H NMR (600 MHz, 25 ºC, C_6D_6): 1.01 (d, J_{HP}= 6.2 Hz, 9H, PMe_3), 1.43 (s, 18H, *t*Bu), 1.48 (s, 18H, *t*Bu), 2.26 (s, 2H, $ZrCH_2Bn$), 3.38 (s, 2H, $NCCH_2Bn$), 6.58 (d, J_{HH} = 7.5 Hz, 2H, CH_{Ph}), 6.69 (m, 1H, CH_{Ph}), 6.74 (m, 1H, CH_{Ph}), 6.78 (m, 2H, CH_{Ph}), 6.80 (m, 2H, $CH_{Arbackbone}$), 6.92-6.98 (m, 4H, CH_{Ph}), 7.17 (m, 2H, $CH_{Arbackbone}$), 7.38 (d, J_{HH} = 2.4 Hz, 2H, CH_{ArO}), 7.72 (d, J_{HH} = 2.4 Hz, 2H, CH_{ArO}). ^{13}C NMR (151 MHz, 25 ºC, C_6D_6): 13.1 (d, J_{CP} = 13.3 Hz, PMe_3), 29.9 (s, CH_{tBu}), 32.1 (s, CH_{tBu}), 34.2 (s, $NCCH_2$), 34.6 (s, $C_{t}Bu$), 35.3 (s, $C_{t}Bu$), 57.2 (s, $ZrCH_2$), 112.7 (s, $CH_{Arbackbone}$), 117.6 (s, CH_{ArO}), 121.2 (s, CH_{Ph}), 121.4 (s, CH_{ArO}), 123.0 (s, $CH_{Arbackbone}$), 125.0 (s, CH_{Ph}), 127.8 (s, CH_{Ph}), 128.1 (s, CH_{Ph}), 128.4 (s, C), 128.6 (s, C), 129.1 (s, CH_{Ph}), 129.4 (s, CH_{Ph}), 130 (s, C), 136.7 (s, C), 139.4 (s, C), 141.1 (s, C), 147.5 (s, C), 159.16 (d, J_{CP} = 5.2 Hz, N*C*N). Signals for quaternary carbons are missing, probably overlapping with those of the benzene-d_6 ^{31}P (162 MHz, 25 ºC, C_6D_6): -34.49 (s, PMe_3). Anal. Calcd. for $C_{52}H_{67}N_2O_2PZr$: C, 71.44; H, 7.72; N, 3.20. Found: C, 70,80; H, 7.41; N, 3.59.

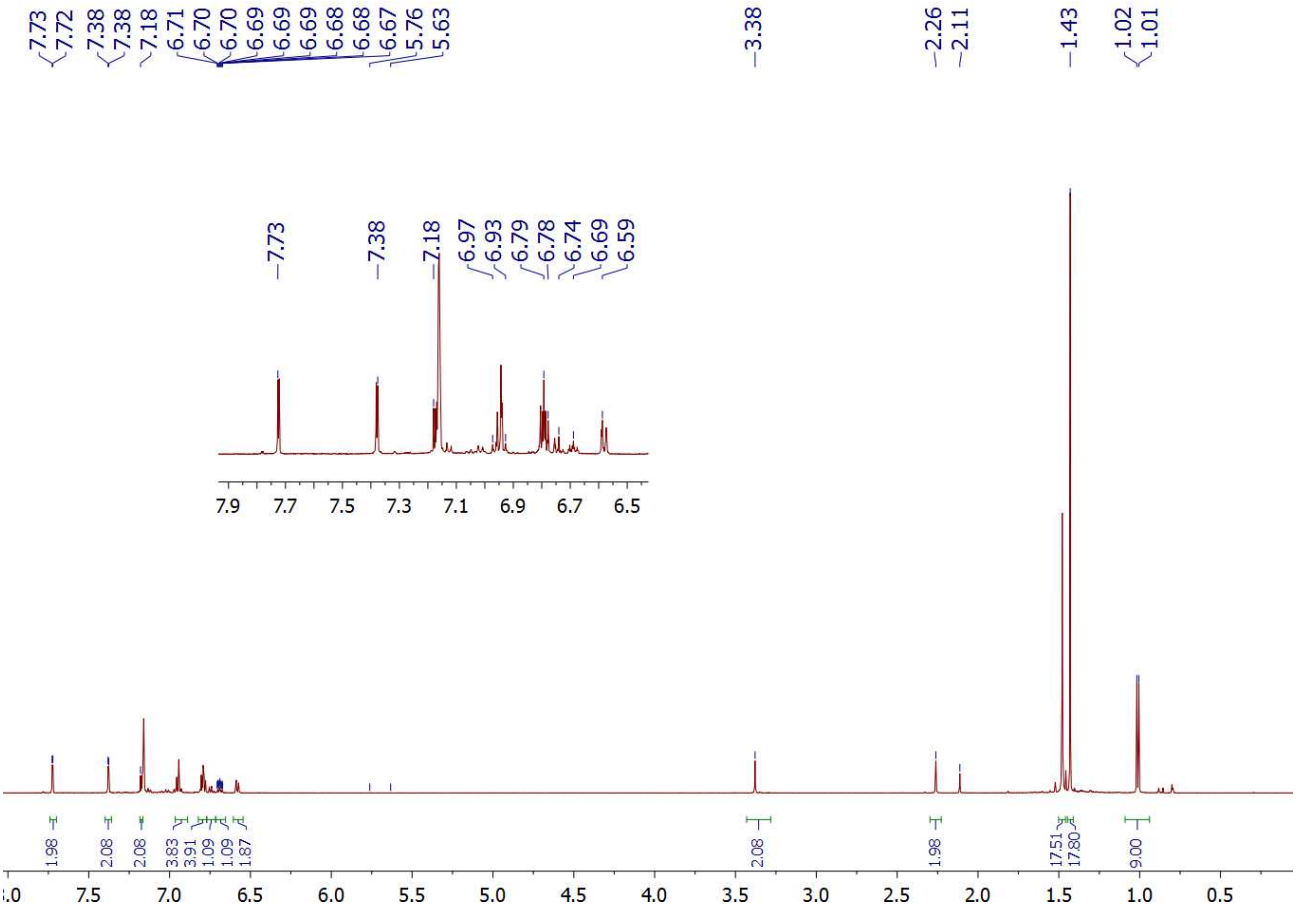

Figure S1. ^{1}H NMR in benzene-d_6 of complex **2** at 25 °C (with some trace of toluene).

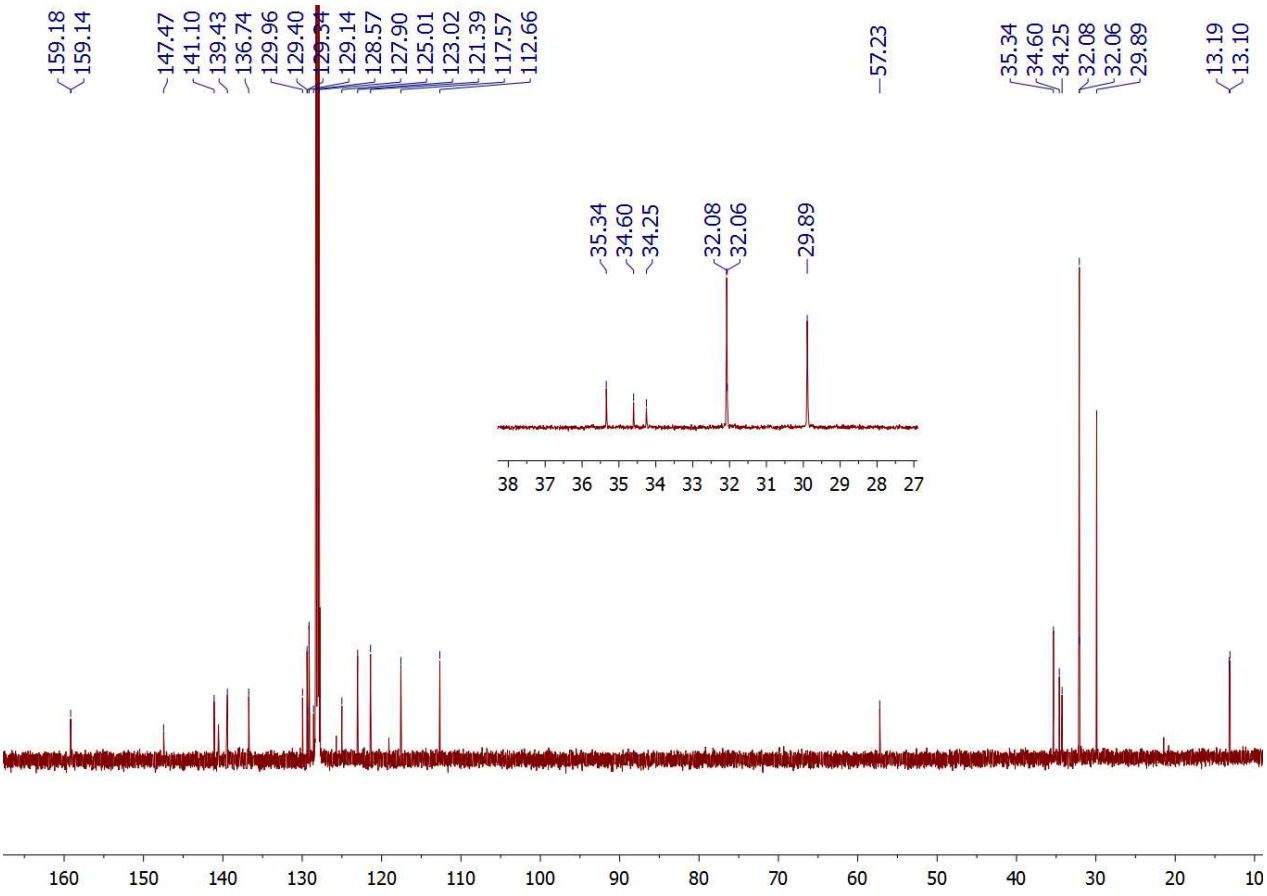

Figure S2. ^{13}C NMR in benzene-*d*$_6$ of complex **2** at 25 °C (with some trace of toluene).

Reaction of Ni(COD)$_2$ with an excess of PMe$_3$: In a J-Young NMR tube, an excess of trimethylphosphine was added to a solution of Ni(COD)$_2$ (20 mg, 0.073 mmol) in benzene-*d*$_6$. The reaction was monitored by NMR allowing the characterization of Ni(PMe$_3$)$_4$.

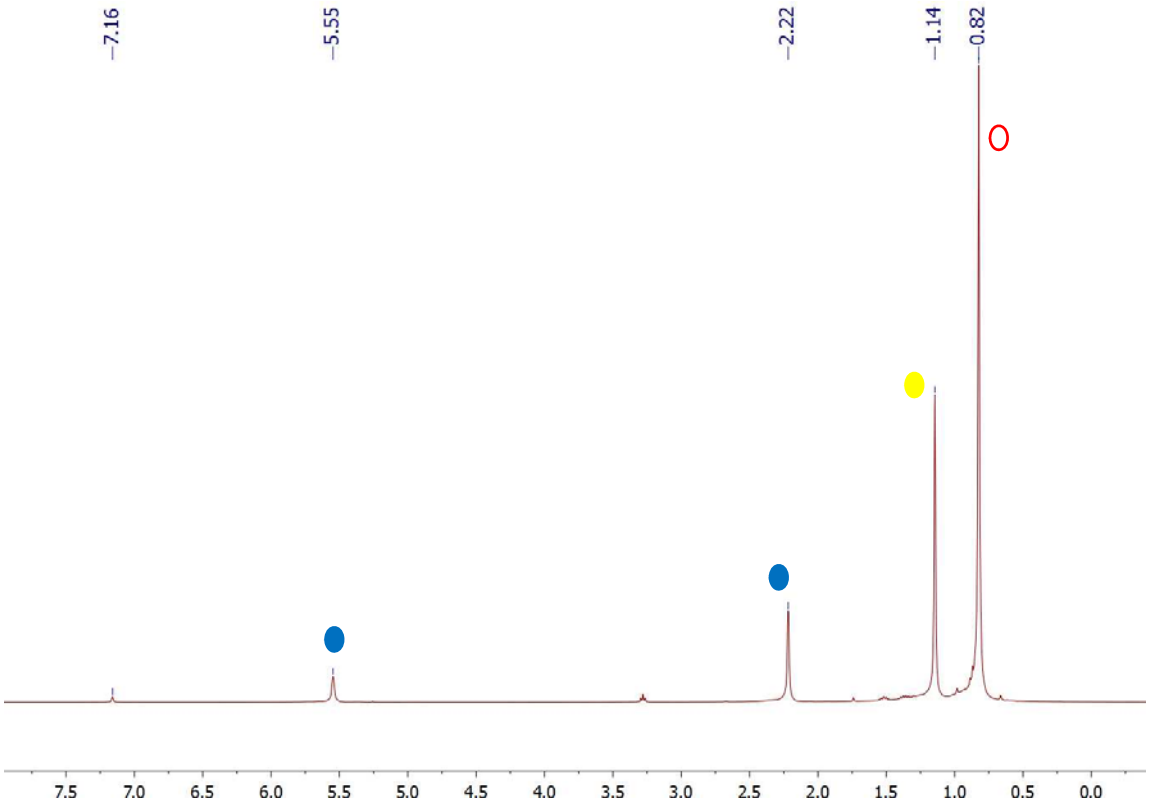

Figure S3. ^{1}H NMR of Ni(PMe$_3$)$_4$ in benzene-*d*$_6$: ● Free COD, ● Ni(PMe$_3$)$_4$, ○ Free PMe$_3$.

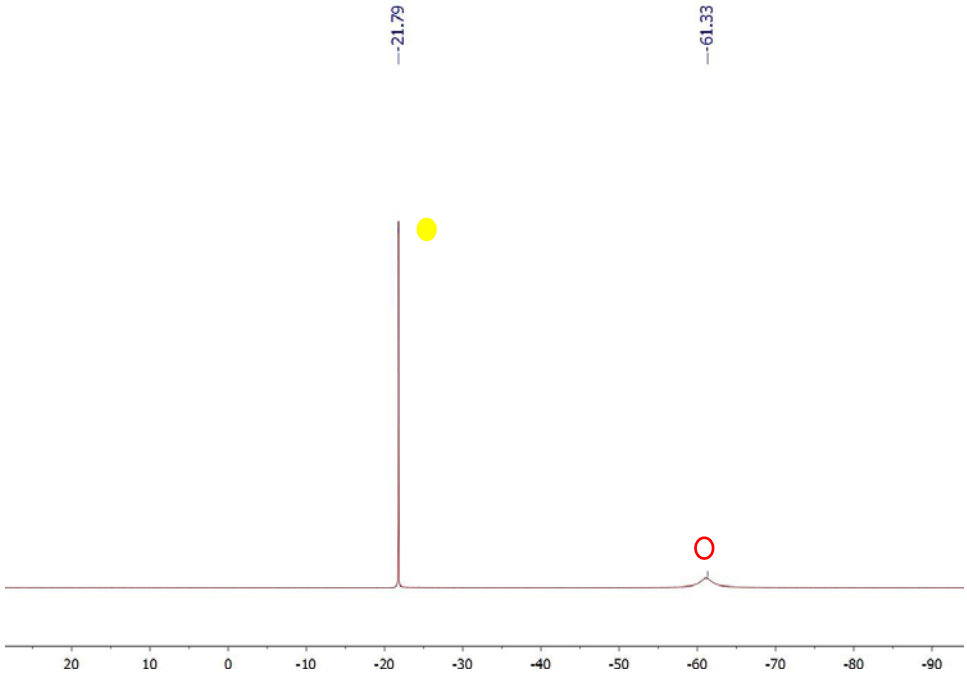

Figure S4. ^{31}P NMR of Ni(PMe$_3$)$_2$ in benzene-*d*$_6$: ● Ni(PMe$_3$)$_2$, ○ Free PMe$_3$.

Reaction of $Ni(COD)_2$ with 1.5 equivalent of PMe_3: In a J-Young NMR tube, 1.5 equivalent of trimethylphosphine (11 µL, 0.11 mmol) was added to a solution of $Ni(COD)_2$ (20 mg, 0.073 mmol) in benzene-d_6 yielding a mixture of $Ni(COD)(PMe_3)_2$ and $Ni(PMe_3)_4$.

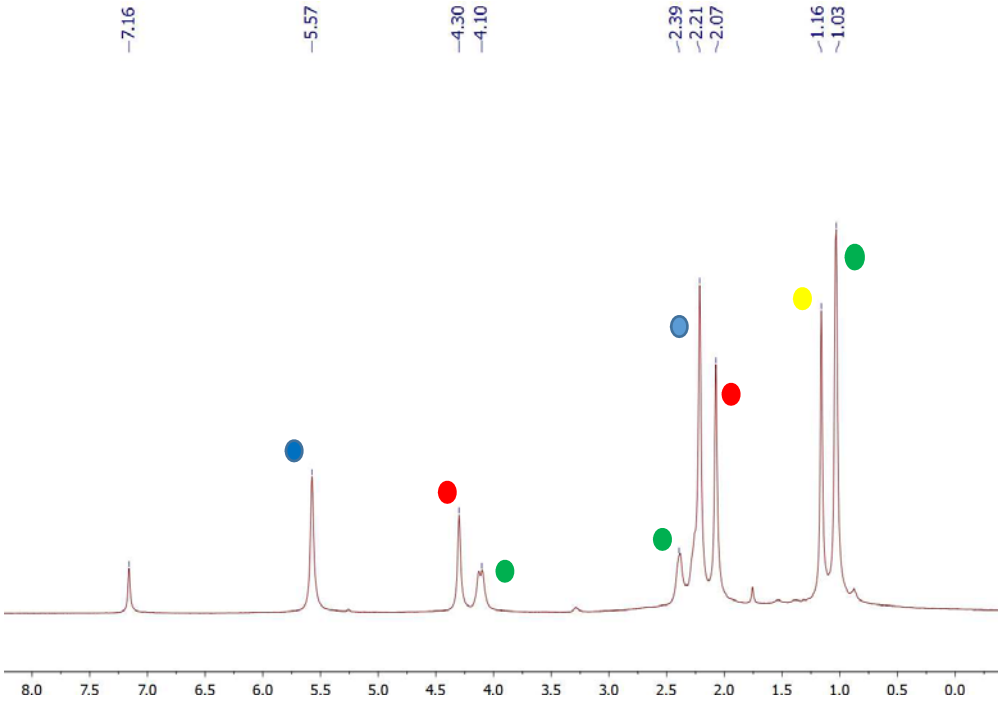

Figure S5. ^1H NMR the reaction of $Ni(COD)_2$ with 1.5 equiv. of PMe_3 in benzene-d_6: ● Free COD, ● $Ni(PMe_3)_4$, ● $Ni(COD)_2$, ● $Ni(COD)(PMe_3)_2$.

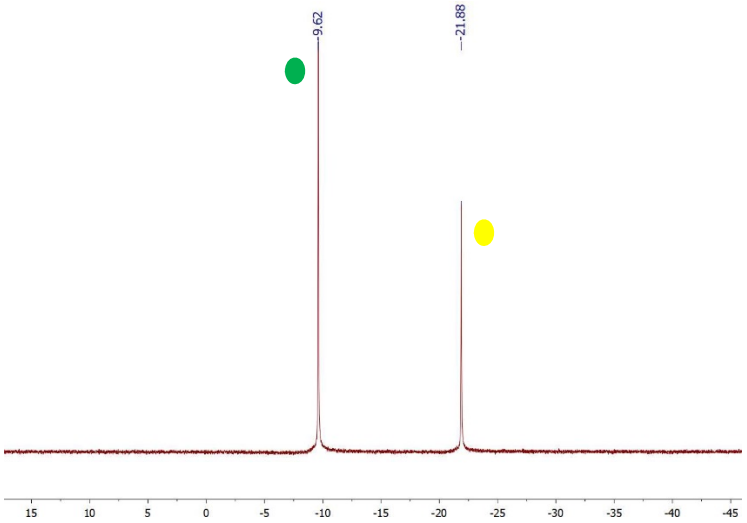

Figure S6. ^{31}P NMR the reaction of $Ni(COD)_2$ with 1.5 equiv. of PMe_3 in benzene-d_6: ● $Ni(PMe_3)_4$, ● $Ni(COD)(PMe_3)_2$.

Reaction of complex 2 with Ni(COD)$_2$: In a J-Young NMR tube, a solution of Ni(COD)$_2$ (4 mg, 0.014 mmol) in benzene-*d*$_6$ (0.3 mL) is added to a solution of complex **2** (25 mg, 0.028 mmol) in benzene-*d*$_6$ (0.4 mL).

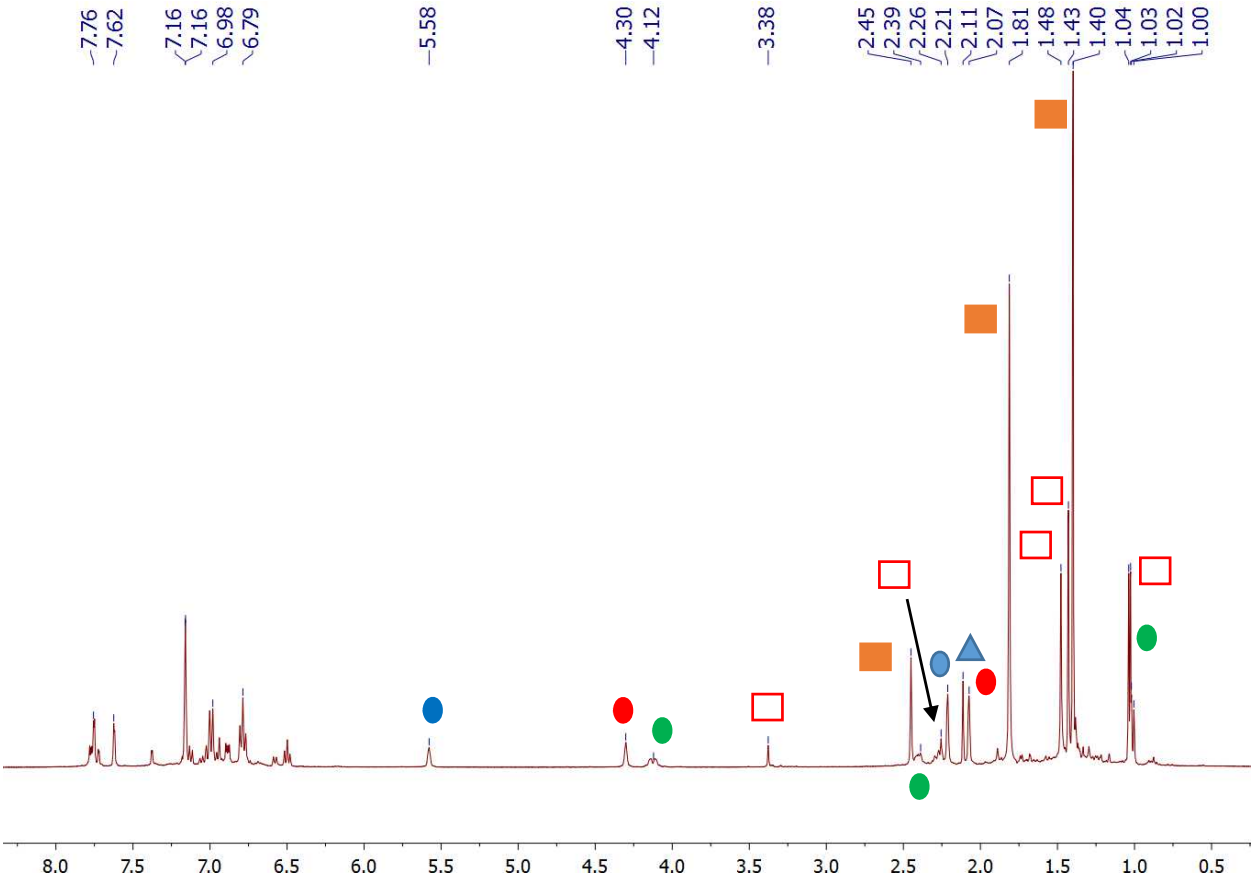

Figure S7. ^{1}H NMR of the reaction of complex **2** with Ni(COD)$_2$ after one night at room temperature: ● Free COD, ● Ni(COD)$_2$, ● Ni(COD)(PMe$_3$)$_2$, ■ complex **1**, □ complex **2**, ▲ toluene.

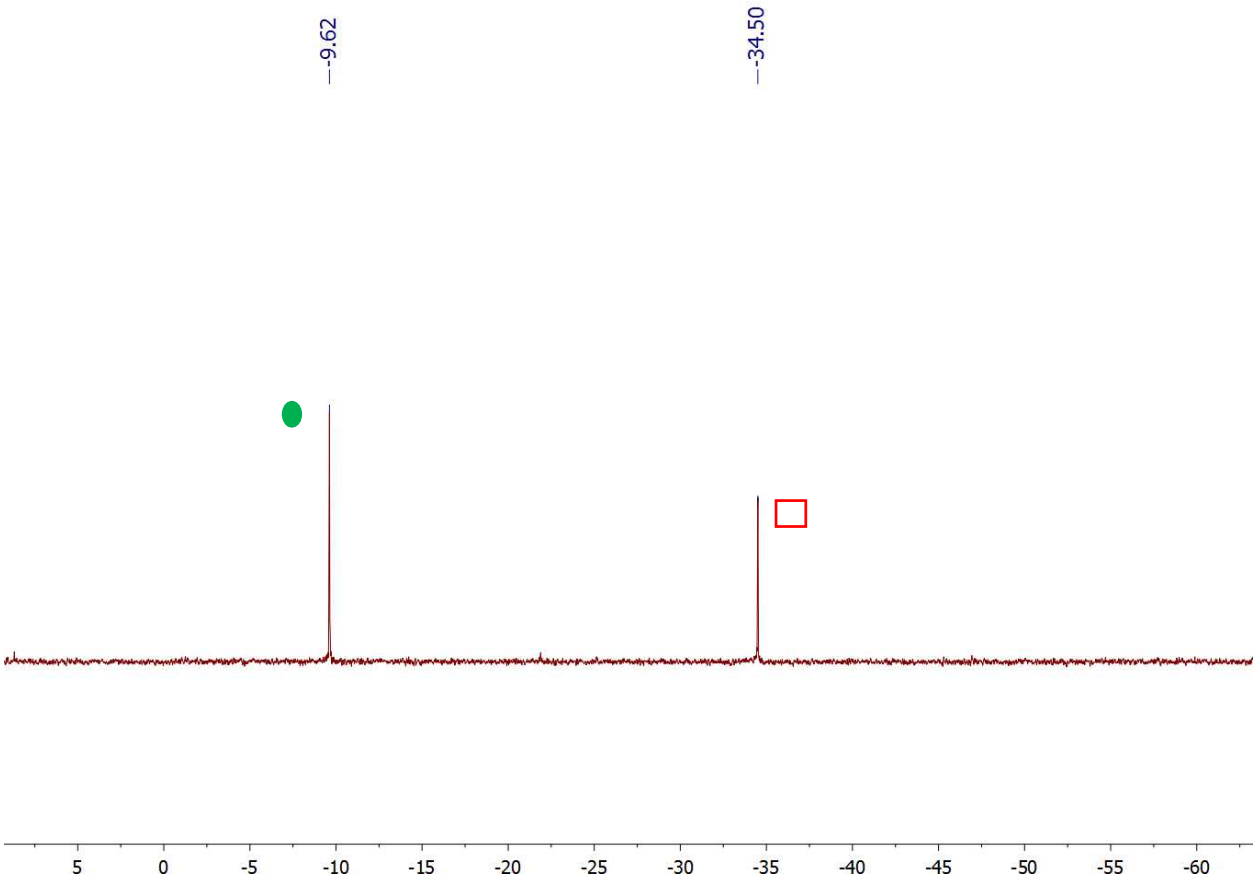

Figure S8. ^{31}P NMR of the reaction of complex **2** with $Ni(COD)_2$ after on night at room temperature: ● $Ni(COD)(PMe_3)_2$, □ complex **2**.

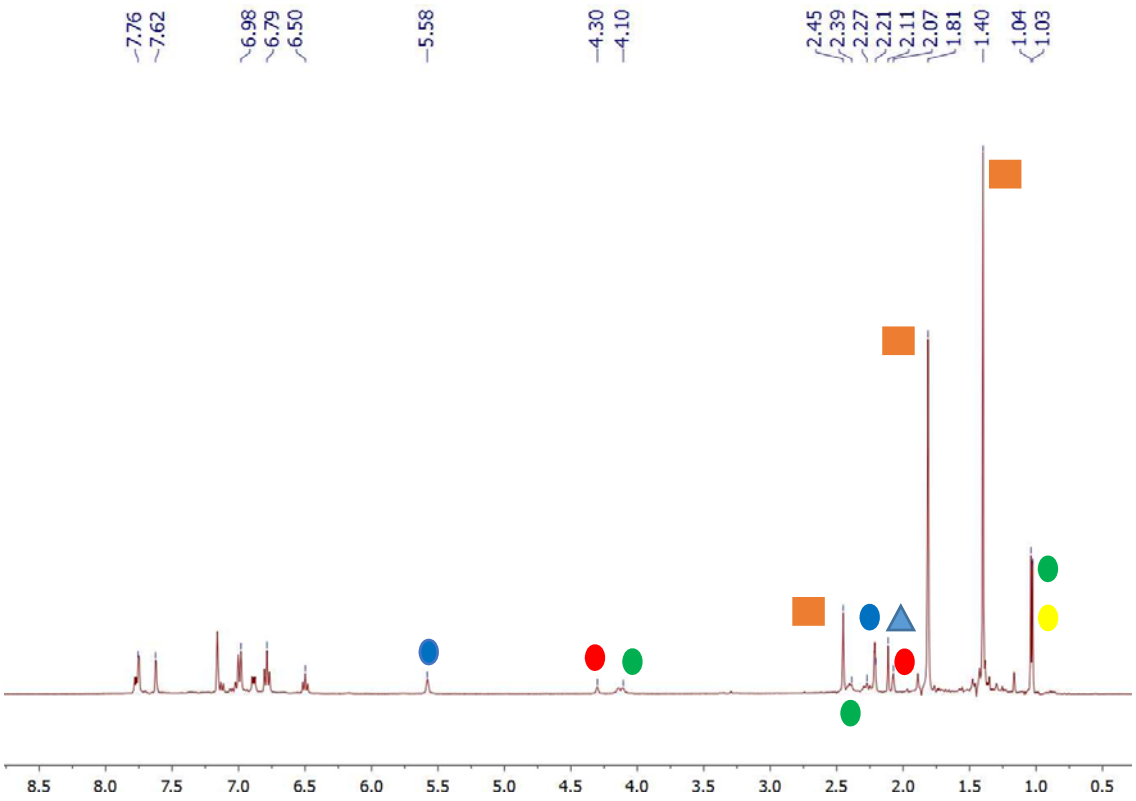

Figure S9. ^{1}H NMR of the reaction of complex **2** with Ni(COD)$_2$ after one hour at 50 °C: Free COD, Ni(COD)$_2$, Ni(COD)(PMe$_3$)$_2$, Ni(PMe$_3$)$_4$, complex **1**, toluene.

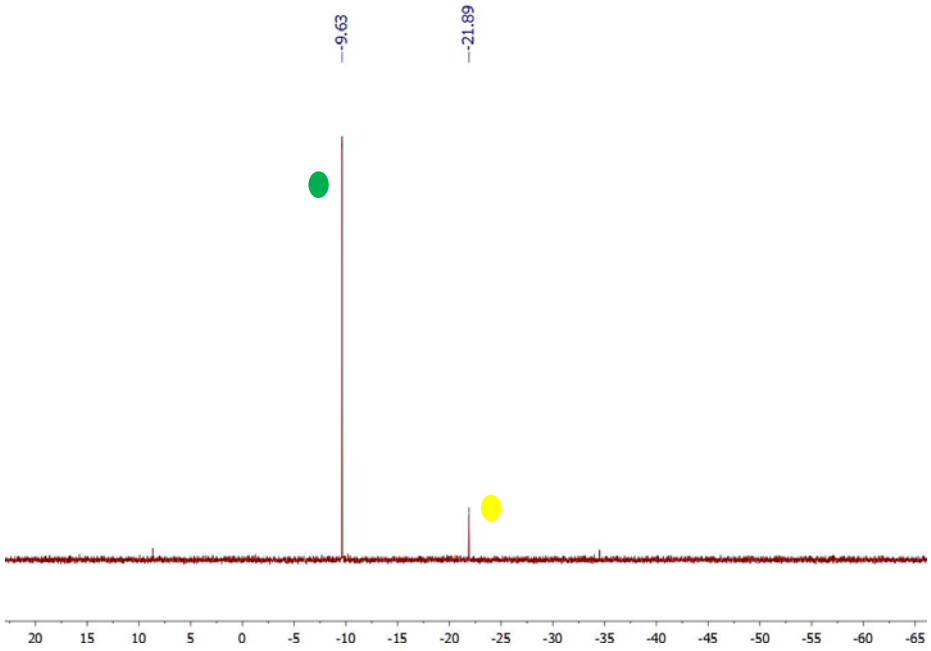

Figure S10. ^{31}P NMR of the reaction of complex **2** with Ni(COD)$_2$ after one hour at 50 °C: Ni(COD)(PMe$_3$)$_2$, Ni(PMe$_3$)$_4$.

Reaction of complex 2 with BPh_3: In a J-Young NMR tube, a solution of BPh_3 (7 mg, 0.028 mmol) in benzene-d_6 (0.3 mL) is added to a solution of complex **2** (25 mg, 0.028 mmol) in benzene-*d_6* (0.4 mL).

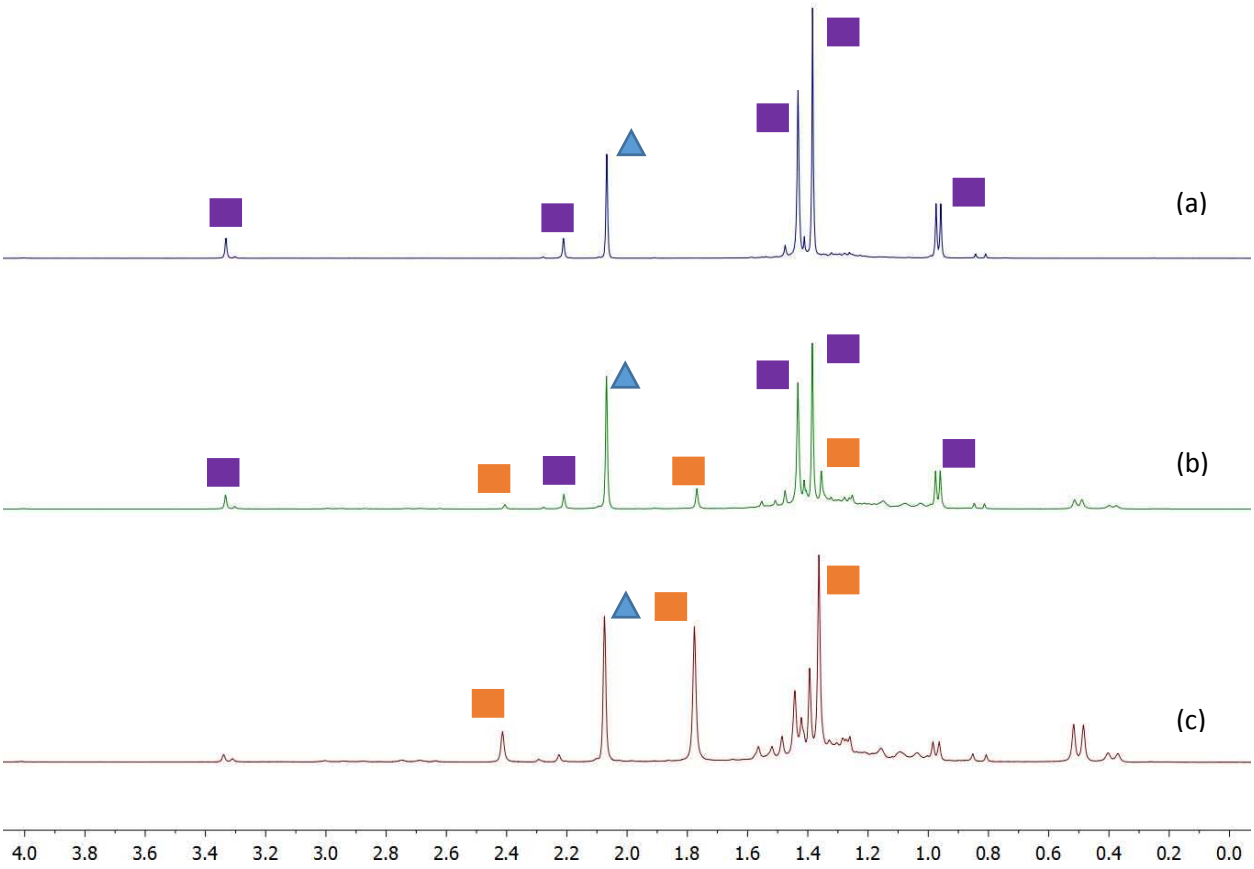

Figure S11. ^1H NMR of the reaction of complex **2** with BPh_3 in benzene-*d_6* at rt: (a) before addition of BPh_3, (b) after 30 minutes at room temperature, (c) overnight at room temperature : ■ complex **2**, ■ complex **1**, ▲ toluene.

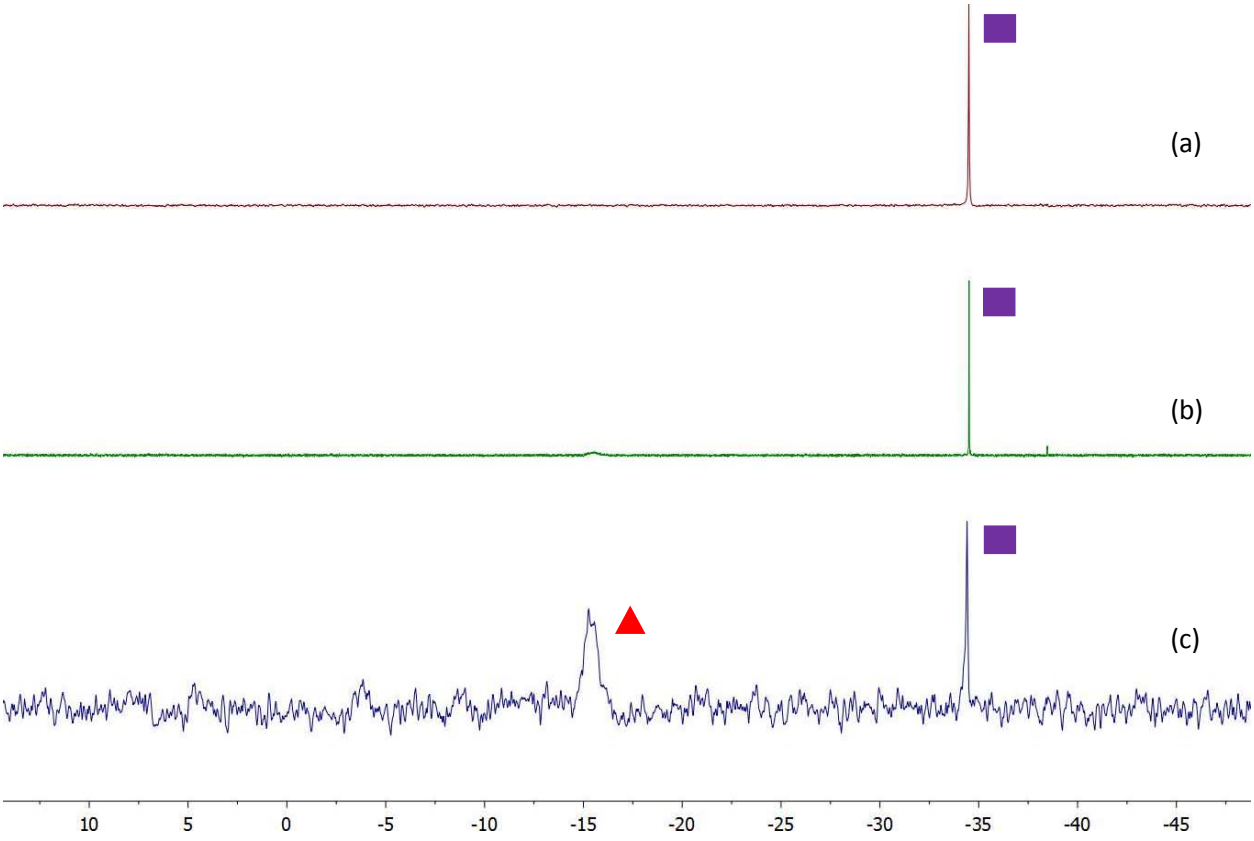

Figure S12. ^{31}P NMR of the reaction of complex **2** with BPh_3 in benzene-d_6 at rt: (a) before addition of BPh_3, (b) after 30 minutes at room temperature, (c) overnight at room temperature: ■ complex **2**, ▲ Ph_3B-PMe_3.

Synthesis of dimer 3: Complex **1** (15 mg, 0.018 mmol) was dissolved in 1 mL of benzene or toluene and then the solution was degassed. An atmosphere of ammonia was introduced in the flask and the mixture was stirred during 3h at room temperature. The solution is then evaporated to dryness to yield quantitatively complex **3** as a yellow powder. ^1H (500 MHz, 25 ºC, C_6D_6): 0.34 (br s, NH_3), 1.27 (s, 18H, *t*Bu), 1.42 (s, 18H, *t*Bu), 1.44 (s, 2H, NH_2), 3.46 (s, 2H, CH_{2Bn}), 5.89 (m, 2H, CH_{Ph}), 6.67 (m, 3H, CH_{Ph}), 6.89 (m, 2H, $CH_{Arbackbone}$), 7.08 (m, 2H, $CH_{Arbackbone}$), 7.36 (d, J_{HH} = 2.4 Hz, 2H, CH_{ArO}), 7.58 (d, J_{HH} = 2.4 Hz, 2H, CH_{ArO}). ^{13}C NMR (100.62 MHz, 25 ºC, C_6D_6): 30.2 (*t*Bu), 32.2 (*t*Bu), 33.8 ($NCCH_2$), 34.5 (*t*Bu), 35.1 (*t*Bu), 112.4 (CH), 118.3 (CH), 119.5 (C), 121.4 (CH), 122.5 (CH), 125.3 (CH), 128.4 (CH), 129.0 (CH), 130.3 (C), 136.9 (C), 138.1 (C),

141.4 (C), 143.6 (C), 159.8 (C). Anal. Calcd. for $C_{84}H_{112}N_8O_4Zr_2$: C, 68.16; H, 7.63; N, 7.57. Found: C, 68.44; H, 7.61; N, 3.23. (This compound is air- and moisture-sensitive, and despite repeated attempts satisfactory %N analysis could not be obtained.)

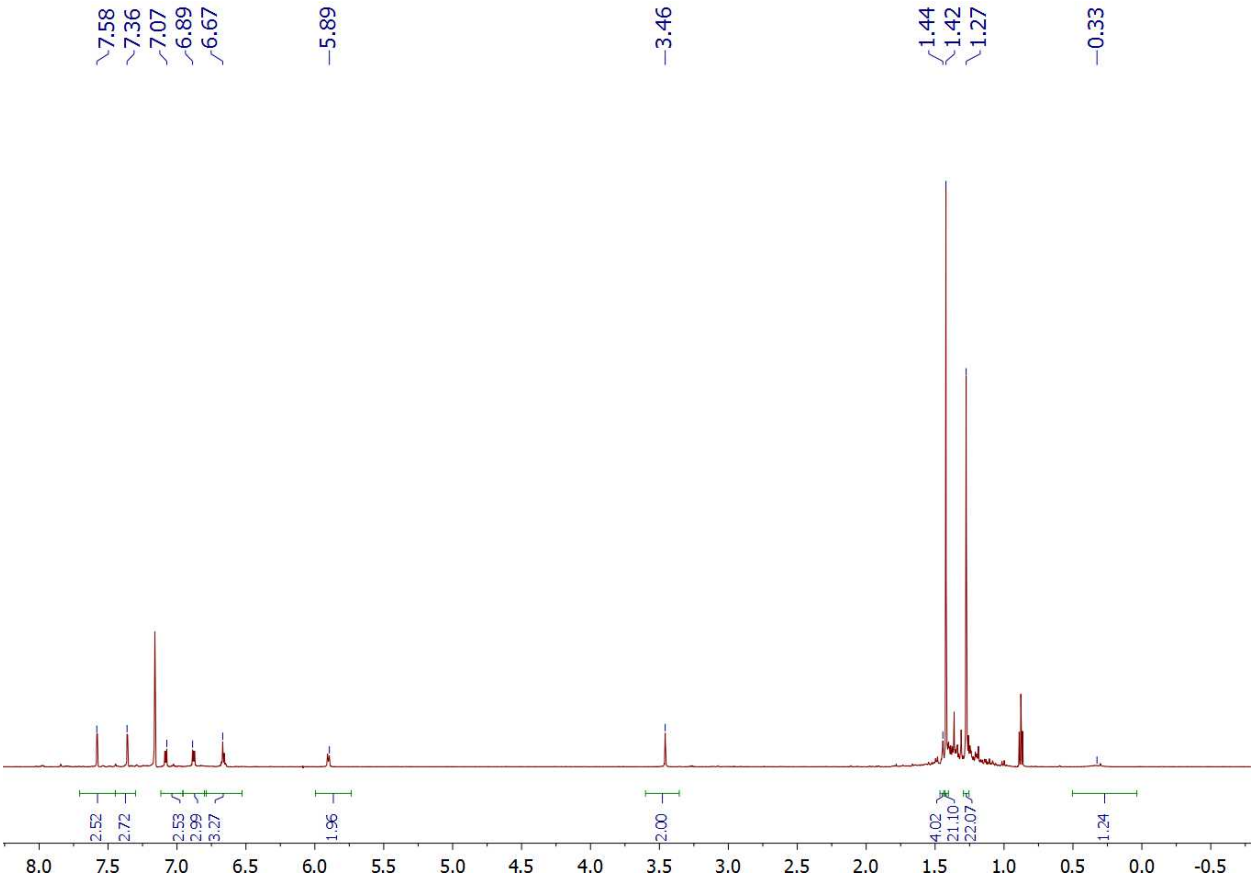

Figure S13. ^{1}H NMR of complex **3** in benzene-*d*$_6$ at 25 °C (presence of pentane).

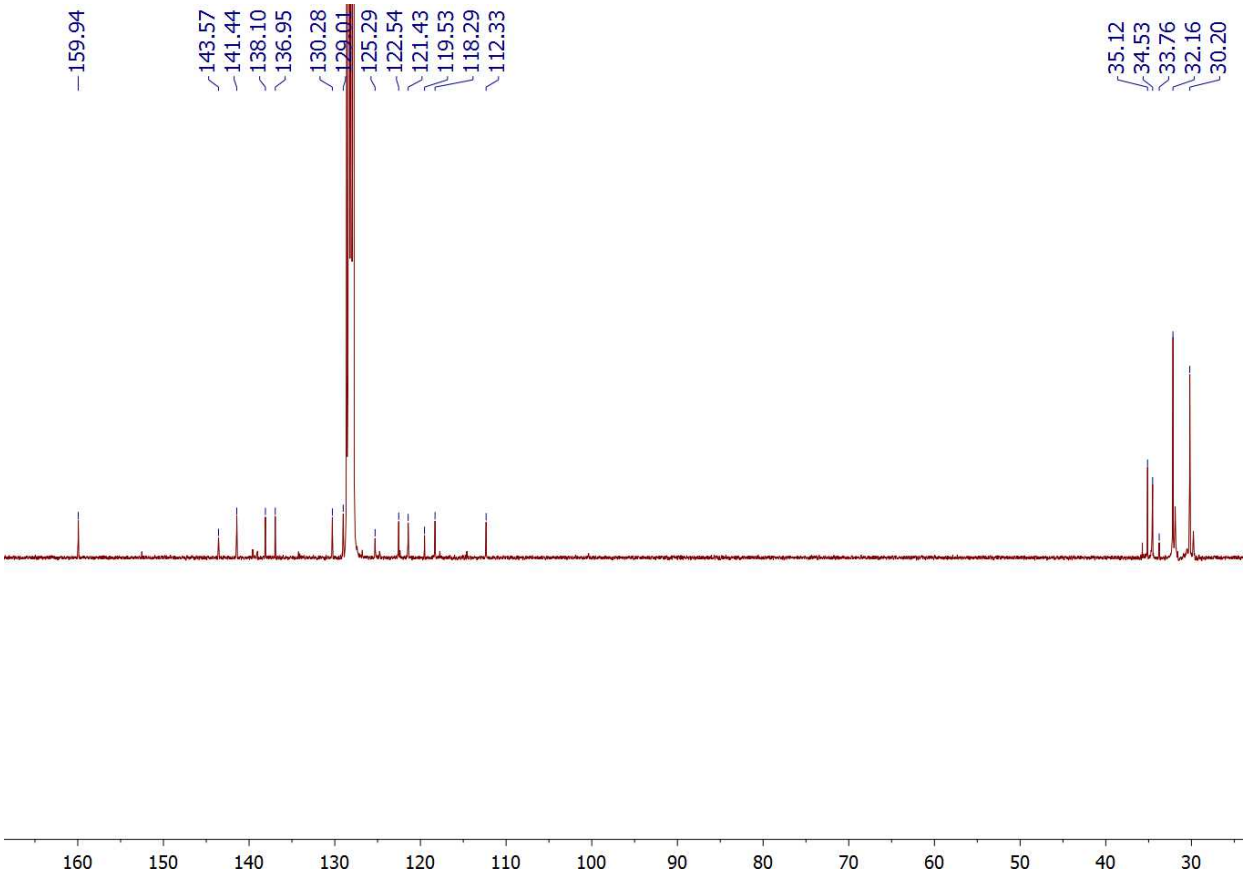

Figure S14: ^{13}C NMR of complex **3** in benzene-d_6 at 25 °C.

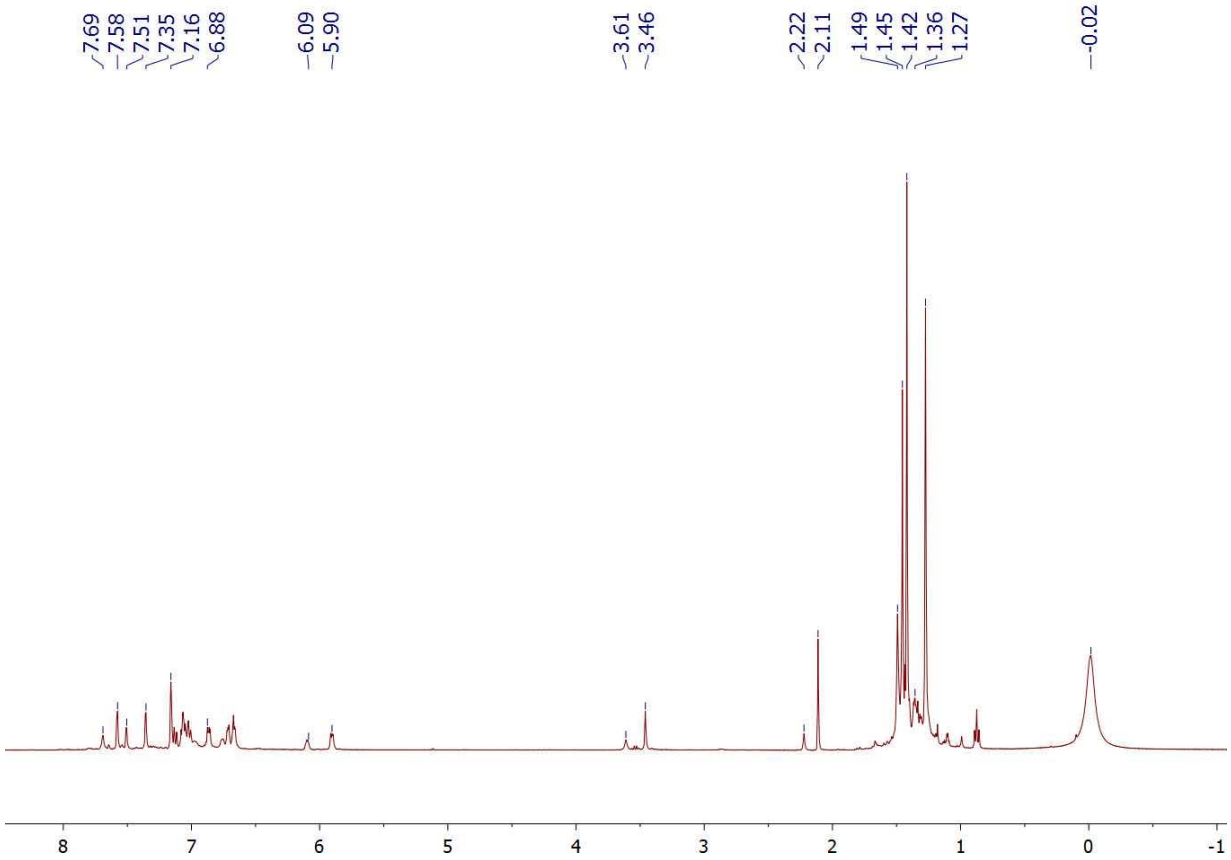

Figure S15. ^{1}H NMR of the mixture of complex **1** with ammonia after 30 minutes at rt in benzene-*d*$_6$ at 25 °C (presence of ether and pentane).

Complex 4: In a J-Young NMR tube, complex **1** (15 mg, 0.018 mmol) was dissolved in 0.8 mL of toluene-*d*$_8$. The NMR tube was degassed and cooled at -60 °C, then an atmosphere of ammonia was introduced. At -60 °C, two products are observed. Major: ^{1}H NMR (500 MHz, -60 ºC, toluene-*d*$_8$): -0.05 (br s, NH_3), 1.50 (s, 18H, *t*Bu), 1.53 (s, 18H, *t*Bu), 2.32 (s, 2H, CH_{2Bn}), 3.73 (s, 2H, CH_{2Bn}), 6.08 (m, 2H, CH_{Ph}), 6.66 (m, 3H, CH_{Ph}), 6.72 (m, 1H, CH_{Ph}), 6.78 (m, 2H, $CH_{Arbackbone}$), 7.06 (m, 4H, CH_{Ph}), 7.11 (m, 2H, $CH_{Arbackbone}$), 7.57 (s, 2H, CH_{ArO}), 7.77 (s, 2H, CH_{ArO}). ^{13}C NMR (121 MHz, -60 ºC, toluene-*d*$_8$): 29.7 (*t*Bu), 32.1 (*t*Bu), 33.4 (NC*C*H_2), 34.6 (*t*Bu), 35.3 (*t*Bu), 52.2 (Zr*C*H_2), 112.7 ($CH_{Arbackbone}$), 119.1 (CH_{ArO}), 121.4 (CH_{ArO}), 122.9 ($CH_{Arbackbone}$), 125.1 (CH_{Ph}), 125.4 (CH_{Ph}), 128.2 (CH_{Ph}), 128.4 (CH_{Ph}), 128.6 (CH_{Ph}), 129.0 (CH_{Ph}), 130.3 (C), 136.2 (C), 138.0 (C), 141.2 (C), 143.8 (C), 156.8 (C), 159.8 (C). Minor: ^{1}H NMR (500 MHz, -60 ºC, toluene-*d*$_8$): 1.47 (s, 18H, *t*Bu), 1.75 (s, 18H, *t*Bu), 2.28 (s, 2H, CH_{2Bn}), 3.47 (s, 2H, CH_{2Bn}), 6.12 (d, J_{HH} = 7.4 Hz, 2H, CH_{Ph}), 6.60 (m, 2H, $CH_{Arbackbone}$), 6.70 (m, 2H, CH_{Ph}), 6.94 (m, 2H, $CH_{Arbackbone}$), 7.01 (m,

2H, CH_{Ph}), 7.14 (m, 2H, CH_{Ph}), 7.53 (s, 2H, CH_{ArO}), 7.63 (s, 2H, CH_{ArO}). ^{13}C NMR (121 MHz, -60 ºC, toluene-d_8): 30.0 (*t*Bu), 31.7 (*t*Bu), 34.5(*t*Bu), 35.4 ($NCCH_2$), 54.2 ($ZrCH_2$), 110.7 ($CH_{Arbackbone}$), 117.2 ($CH_{Arbackbone}$), 118.2 (CH_{ArO}), 121.2 (CH_{ArO}), 129.3 (CH_{Ph}). Not all the ^{13}C NMR signals could be observed for the minor product due to their overlap with other signals combined with their low intensity.

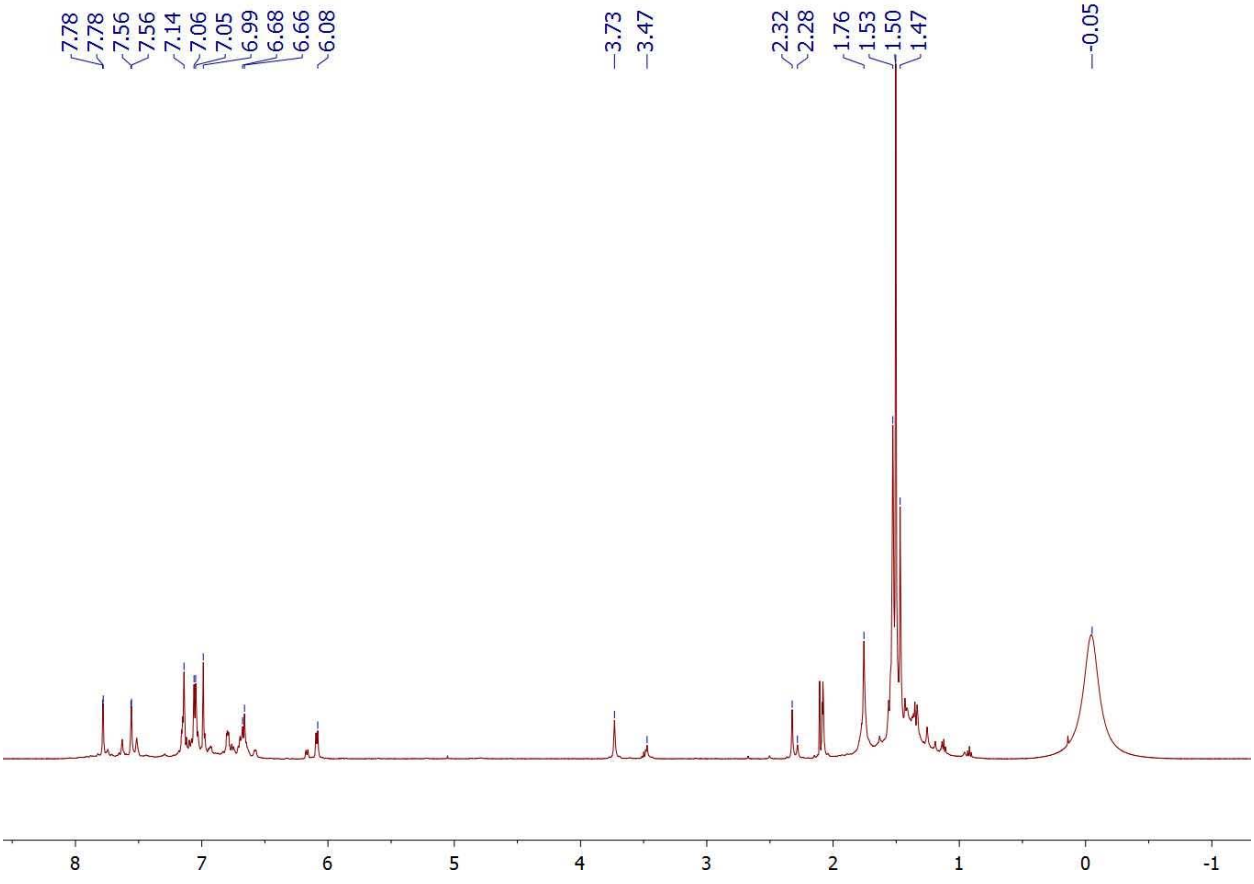

Figure S16: ^1H NMR of complexes **4** in toluene-d_8 at -60 °C (presence of ether).

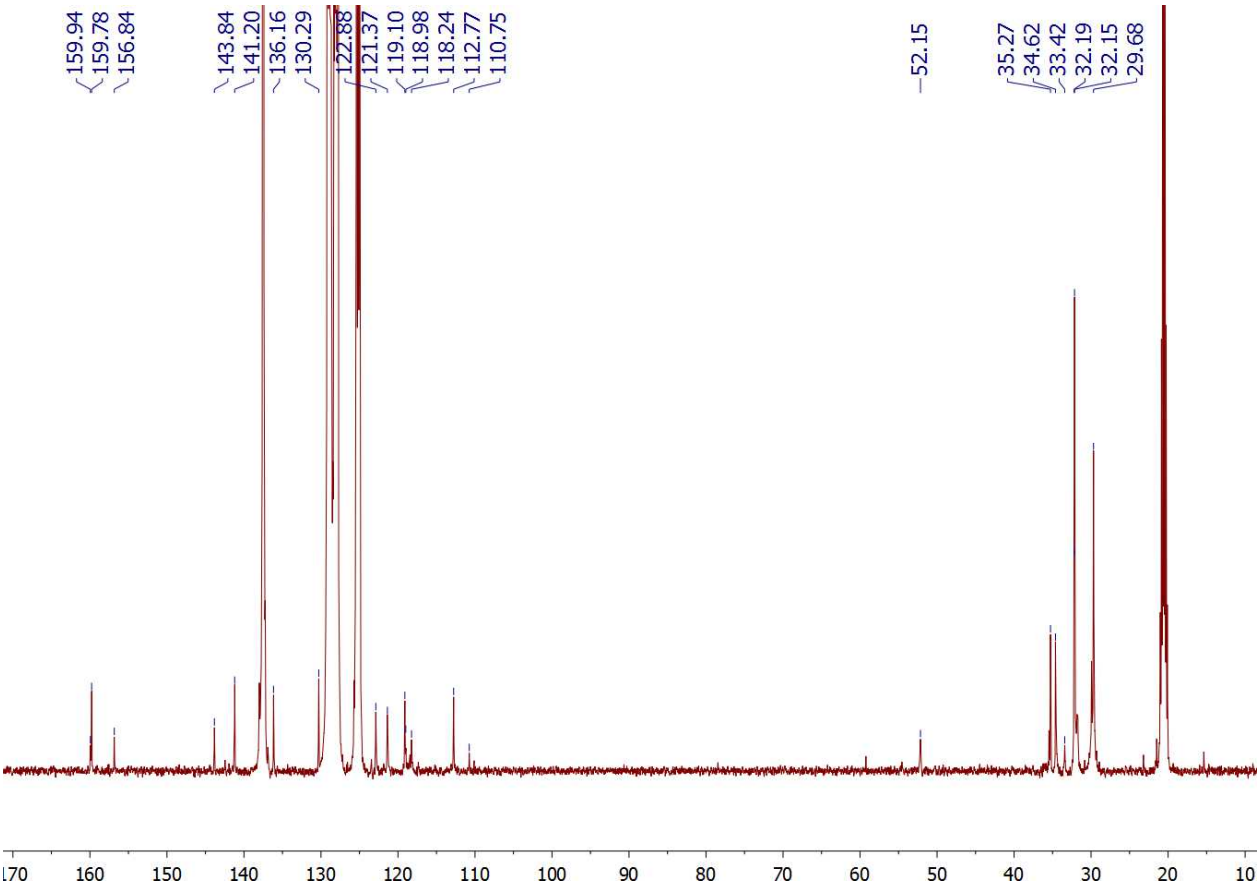

Figure S17: ^{13}C NMR of complex **4** in toluene-d_8 at -60 °C (presence of ether).

2. Crystallographic data:

a) Complex 2 (CCDC 1404595):

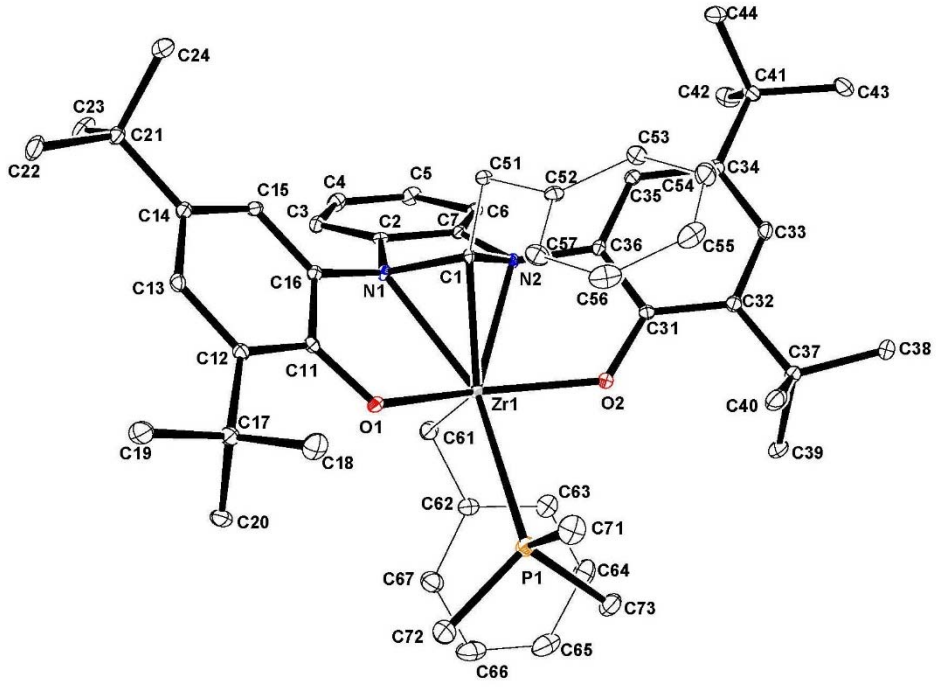

Figure S18: Molecular structure of complex **2**. For clarity, the hydrogen atoms were omitted.

Table 1. Crystal data and structure refinement for complex **2**.

Empirical formula	C52 H67 N2 O2 P Zr	
Formula weight	874.26	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.2090(7) Å	α= 90°.
	b = 11.0430(4) Å	β= 96.8727(15)°.
	c = 22.7466(10) Å	γ = 90°.
Volume	4790.5(3) $Å^3$	
Z	4	
Density (calculated)	1.212 Mg/m^3	
Absorption coefficient	0.303 mm^{-1}	

F(000)	1856
Crystal size	0.300 x 0.100 x 0.050 mm^3
Theta range for data collection	2.363 to 33.153°.
Index ranges	-27<=h<=29, -16<=k<=16, -34<=l<=34
Reflections collected	99225
Independent reflections	18233 [R(int) = 0.0967]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7474 and 0.6799
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18233 / 0 / 538
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.0931
R indices (all data)	R1 = 0.1163, wR2 = 0.1085
Extinction coefficient	n/a
Largest diff. peak and hole	1.199 and -0.574 $e.Å^{-3}$

Experimental details:

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Mo K_α radiation (λ = 0.71073 Å) from an IμS micro-source for the structure of compound **2**. The structure was solved by direct methods using SHELXS[3] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[4] using established refinement techniques.[5] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups).

Compound **2** crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit. The highest residual density are located in positions consistent with the phosphorus and oxygen atoms from a partially occupied $OPMe_3$. A disordered model was attempted, however, the refinement was not stable possibly due to the small occupancy of the presumed $OPMe_3$ (<5%).

Table 2. Bond lengths [Å] and angles [°] for complex **2**.

Zr(1)-O(2)	2.0703(12)	C(56)-H(56)	0.9500
Zr(1)-O(1)	2.0714(13)	C(57)-H(57)	0.9500
Zr(1)-C(1)	2.1678(17)	N(1)-C(16)	1.425(2)
Zr(1)-C(61)	2.2770(19)	N(1)-C(2)	1.434(2)
Zr(1)-N(2)	2.4266(15)	O(1)-C(11)	1.355(2)
Zr(1)-N(1)	2.4352(15)	C(11)-C(16)	1.408(3)
Zr(1)-P(1)	2.8454(6)	C(11)-C(12)	1.412(3)
P(1)-C(73)	1.815(2)	C(12)-C(13)	1.404(3)
P(1)-C(72)	1.823(2)	C(12)-C(17)	1.536(3)
P(1)-C(71)	1.824(2)	C(17)-C(19)	1.534(3)
C(71)-H(71A)	0.9800	C(17)-C(20)	1.537(3)
C(71)-H(71B)	0.9800	C(17)-C(18)	1.541(3)
C(71)-H(71C)	0.9800	C(18)-H(18A)	0.9800
C(72)-H(72A)	0.9800	C(18)-H(18B)	0.9800
C(72)-H(72B)	0.9800	C(18)-H(18C)	0.9800
C(72)-H(72C)	0.9800	C(19)-H(19A)	0.9800
C(73)-H(73A)	0.9800	C(19)-H(19B)	0.9800
C(73)-H(73B)	0.9800	C(19)-H(19C)	0.9800
C(73)-H(73C)	0.9800	C(20)-H(20A)	0.9800
C(1)-N(2)	1.488(2)	C(20)-H(20B)	0.9800
C(1)-N(1)	1.489(2)	C(20)-H(20C)	0.9800
C(1)-C(51)	1.512(2)	C(13)-C(14)	1.393(3)
C(51)-C(52)	1.514(3)	C(13)-H(13)	0.9500
C(51)-H(51A)	0.9900	C(14)-C(15)	1.396(3)
C(51)-H(51B)	0.9900	C(14)-C(21)	1.533(3)
C(52)-C(53)	1.388(3)	C(15)-C(16)	1.381(2)
C(52)-C(57)	1.396(3)	C(15)-H(15)	0.9500
C(53)-C(54)	1.393(3)	C(21)-C(22)	1.530(3)
C(53)-H(53)	0.9500	C(21)-C(23)	1.534(3)
C(54)-C(55)	1.377(3)	C(21)-C(24)	1.538(3)
C(54)-H(54)	0.9500	C(22)-H(22A)	0.9800
C(55)-C(56)	1.385(3)	C(22)-H(22B)	0.9800
C(55)-H(55)	0.9500	C(22)-H(22C)	0.9800
C(56)-C(57)	1.388(3)	C(23)-H(23A)	0.9800

C(23)-H(23B)	0.9800	C(34)-C(35)	1.393(3)
C(23)-H(23C)	0.9800	C(34)-C(41)	1.537(3)
C(24)-H(24A)	0.9800	C(35)-C(36)	1.379(3)
C(24)-H(24B)	0.9800	C(35)-H(35)	0.9500
C(24)-H(24C)	0.9800	C(41)-C(43)	1.532(3)
C(2)-C(3)	1.379(2)	C(41)-C(42)	1.534(3)
C(2)-C(7)	1.392(3)	C(41)-C(44)	1.537(3)
C(3)-C(4)	1.403(3)	C(42)-H(42A)	0.9800
C(3)-H(3)	0.9500	C(42)-H(42B)	0.9800
C(4)-C(5)	1.382(3)	C(42)-H(42C)	0.9800
C(4)-H(4)	0.9500	C(43)-H(43A)	0.9800
C(5)-C(6)	1.403(3)	C(43)-H(43B)	0.9800
C(5)-H(5)	0.9500	C(43)-H(43C)	0.9800
C(6)-C(7)	1.378(3)	C(44)-H(44A)	0.9800
C(6)-H(6)	0.9500	C(44)-H(44B)	0.9800
C(7)-N(2)	1.430(2)	C(44)-H(44C)	0.9800
N(2)-C(36)	1.433(2)	C(61)-C(62)	1.477(3)
O(2)-C(31)	1.357(2)	C(61)-H(61A)	0.9900
C(31)-C(36)	1.404(2)	C(61)-H(61B)	0.9900
C(31)-C(32)	1.411(3)	C(62)-C(67)	1.394(3)
C(32)-C(33)	1.399(3)	C(62)-C(63)	1.415(3)
C(32)-C(37)	1.539(3)	C(63)-C(64)	1.382(3)
C(37)-C(40)	1.535(3)	C(63)-H(63)	0.9500
C(37)-C(38)	1.537(3)	C(64)-C(65)	1.378(4)
C(37)-C(39)	1.544(3)	C(64)-H(64)	0.9500
C(38)-H(38A)	0.9800	C(65)-C(66)	1.374(4)
C(38)-H(38B)	0.9800	C(65)-H(65)	0.9500
C(38)-H(38C)	0.9800	C(66)-C(67)	1.400(3)
C(39)-H(39A)	0.9800	C(66)-H(66)	0.9500
C(39)-H(39B)	0.9800	C(67)-H(67)	0.9500
C(39)-H(39C)	0.9800		
C(40)-H(40A)	0.9800	O(2)-Zr(1)-O(1)	141.65(5)
C(40)-H(40B)	0.9800	O(2)-Zr(1)-C(1)	88.84(6)
C(40)-H(40C)	0.9800	O(1)-Zr(1)-C(1)	87.87(6)
C(33)-C(34)	1.398(3)	O(2)-Zr(1)-C(61)	109.67(6)
C(33)-H(33)	0.9500	O(1)-Zr(1)-C(61)	106.76(6)

C(1)-Zr(1)-C(61)	112.82(7)	H(73A)-C(73)-H(73B)	109.5
O(2)-Zr(1)-N(2)	70.84(5)	P(1)-C(73)-H(73C)	109.5
O(1)-Zr(1)-N(2)	122.43(5)	H(73A)-C(73)-H(73C)	109.5
C(1)-Zr(1)-N(2)	37.27(6)	H(73B)-C(73)-H(73C)	109.5
C(61)-Zr(1)-N(2)	87.96(6)	N(2)-C(1)-N(1)	96.69(13)
O(2)-Zr(1)-N(1)	122.76(5)	N(2)-C(1)-C(51)	118.13(15)
O(1)-Zr(1)-N(1)	71.16(5)	N(1)-C(1)-C(51)	118.88(14)
C(1)-Zr(1)-N(1)	37.17(6)	N(2)-C(1)-Zr(1)	80.85(9)
C(61)-Zr(1)-N(1)	85.69(6)	N(1)-C(1)-Zr(1)	81.22(9)
N(2)-Zr(1)-N(1)	54.46(5)	C(51)-C(1)-Zr(1)	147.67(13)
O(2)-Zr(1)-P(1)	79.84(4)	C(1)-C(51)-C(52)	110.59(14)
O(1)-Zr(1)-P(1)	79.26(4)	C(1)-C(51)-H(51A)	109.5
C(1)-Zr(1)-P(1)	141.46(5)	C(52)-C(51)-H(51A)	109.5
C(61)-Zr(1)-P(1)	105.67(5)	C(1)-C(51)-H(51B)	109.5
N(2)-Zr(1)-P(1)	150.46(4)	C(52)-C(51)-H(51B)	109.5
N(1)-Zr(1)-P(1)	150.31(4)	H(51A)-C(51)-H(51B)	108.1
C(73)-P(1)-C(72)	102.22(11)	C(53)-C(52)-C(57)	118.76(18)
C(73)-P(1)-C(71)	102.98(11)	C(53)-C(52)-C(51)	122.43(17)
C(72)-P(1)-C(71)	102.70(11)	C(57)-C(52)-C(51)	118.76(17)
C(73)-P(1)-Zr(1)	116.13(7)	C(52)-C(53)-C(54)	120.5(2)
C(72)-P(1)-Zr(1)	119.36(8)	C(52)-C(53)-H(53)	119.8
C(71)-P(1)-Zr(1)	111.40(8)	C(54)-C(53)-H(53)	119.8
P(1)-C(71)-H(71A)	109.5	C(55)-C(54)-C(53)	120.3(2)
P(1)-C(71)-H(71B)	109.5	C(55)-C(54)-H(54)	119.8
H(71A)-C(71)-H(71B)	109.5	C(53)-C(54)-H(54)	119.8
P(1)-C(71)-H(71C)	109.5	C(54)-C(55)-C(56)	119.77(19)
H(71A)-C(71)-H(71C)	109.5	C(54)-C(55)-H(55)	120.1
H(71B)-C(71)-H(71C)	109.5	C(56)-C(55)-H(55)	120.1
P(1)-C(72)-H(72A)	109.5	C(55)-C(56)-C(57)	120.2(2)
P(1)-C(72)-H(72B)	109.5	C(55)-C(56)-H(56)	119.9
H(72A)-C(72)-H(72B)	109.5	C(57)-C(56)-H(56)	119.9
P(1)-C(72)-H(72C)	109.5	C(56)-C(57)-C(52)	120.5(2)
H(72A)-C(72)-H(72C)	109.5	C(56)-C(57)-H(57)	119.8
H(72B)-C(72)-H(72C)	109.5	C(52)-C(57)-H(57)	119.8
P(1)-C(73)-H(73A)	109.5	C(16)-N(1)-C(2)	124.69(15)
P(1)-C(73)-H(73B)	109.5	C(16)-N(1)-C(1)	116.45(14)

C(2)-N(1)-C(1)	108.72(14)	C(14)-C(13)-H(13)	118.0
C(16)-N(1)-Zr(1)	110.90(11)	C(12)-C(13)-H(13)	118.0
C(2)-N(1)-Zr(1)	117.94(11)	C(13)-C(14)-C(15)	117.41(17)
C(1)-N(1)-Zr(1)	61.61(8)	C(13)-C(14)-C(21)	123.63(17)
C(11)-O(1)-Zr(1)	125.20(11)	C(15)-C(14)-C(21)	118.96(16)
O(1)-C(11)-C(16)	117.43(16)	C(16)-C(15)-C(14)	120.19(17)
O(1)-C(11)-C(12)	123.98(16)	C(16)-C(15)-H(15)	119.9
C(16)-C(11)-C(12)	118.59(17)	C(14)-C(15)-H(15)	119.9
C(13)-C(12)-C(11)	117.43(17)	C(22)-C(21)-C(14)	112.69(16)
C(13)-C(12)-C(17)	121.45(17)	C(22)-C(21)-C(23)	107.98(16)
C(11)-C(12)-C(17)	121.09(16)	C(14)-C(21)-C(23)	109.41(15)
C(19)-C(17)-C(12)	112.47(16)	C(22)-C(21)-C(24)	108.78(16)
C(19)-C(17)-C(20)	107.51(16)	C(14)-C(21)-C(24)	108.63(15)
C(12)-C(17)-C(20)	109.10(16)	C(23)-C(21)-C(24)	109.30(17)
C(19)-C(17)-C(18)	107.79(17)	C(21)-C(22)-H(22A)	109.5
C(12)-C(17)-C(18)	109.64(16)	C(21)-C(22)-H(22B)	109.5
C(20)-C(17)-C(18)	110.30(17)	H(22A)-C(22)-H(22B)	109.5
C(17)-C(18)-H(18A)	109.5	C(21)-C(22)-H(22C)	109.5
C(17)-C(18)-H(18B)	109.5	H(22A)-C(22)-H(22C)	109.5
H(18A)-C(18)-H(18B)	109.5	H(22B)-C(22)-H(22C)	109.5
C(17)-C(18)-H(18C)	109.5	C(21)-C(23)-H(23A)	109.5
H(18A)-C(18)-H(18C)	109.5	C(21)-C(23)-H(23B)	109.5
H(18B)-C(18)-H(18C)	109.5	H(23A)-C(23)-H(23B)	109.5
C(17)-C(19)-H(19A)	109.5	C(21)-C(23)-H(23C)	109.5
C(17)-C(19)-H(19B)	109.5	H(23A)-C(23)-H(23C)	109.5
H(19A)-C(19)-H(19B)	109.5	H(23B)-C(23)-H(23C)	109.5
C(17)-C(19)-H(19C)	109.5	C(21)-C(24)-H(24A)	109.5
H(19A)-C(19)-H(19C)	109.5	C(21)-C(24)-H(24B)	109.5
H(19B)-C(19)-H(19C)	109.5	H(24A)-C(24)-H(24B)	109.5
C(17)-C(20)-H(20A)	109.5	C(21)-C(24)-H(24C)	109.5
C(17)-C(20)-H(20B)	109.5	H(24A)-C(24)-H(24C)	109.5
H(20A)-C(20)-H(20B)	109.5	H(24B)-C(24)-H(24C)	109.5
C(17)-C(20)-H(20C)	109.5	C(15)-C(16)-C(11)	122.33(17)
H(20A)-C(20)-H(20C)	109.5	C(15)-C(16)-N(1)	122.51(16)
H(20B)-C(20)-H(20C)	109.5	C(11)-C(16)-N(1)	115.11(16)
C(14)-C(13)-C(12)	124.03(18)	C(3)-C(2)-C(7)	121.53(17)

C(3)-C(2)-N(1)	131.32(18)	C(37)-C(38)-H(38A)	109.5
C(7)-C(2)-N(1)	106.65(15)	C(37)-C(38)-H(38B)	109.5
C(2)-C(3)-C(4)	116.98(18)	H(38A)-C(38)-H(38B)	109.5
C(2)-C(3)-H(3)	121.5	C(37)-C(38)-H(38C)	109.5
C(4)-C(3)-H(3)	121.5	H(38A)-C(38)-H(38C)	109.5
C(5)-C(4)-C(3)	121.56(18)	H(38B)-C(38)-H(38C)	109.5
C(5)-C(4)-H(4)	119.2	C(37)-C(39)-H(39A)	109.5
C(3)-C(4)-H(4)	119.2	C(37)-C(39)-H(39B)	109.5
C(4)-C(5)-C(6)	120.96(18)	H(39A)-C(39)-H(39B)	109.5
C(4)-C(5)-H(5)	119.5	C(37)-C(39)-H(39C)	109.5
C(6)-C(5)-H(5)	119.5	H(39A)-C(39)-H(39C)	109.5
C(7)-C(6)-C(5)	117.18(18)	H(39B)-C(39)-H(39C)	109.5
C(7)-C(6)-H(6)	121.4	C(37)-C(40)-H(40A)	109.5
C(5)-C(6)-H(6)	121.4	C(37)-C(40)-H(40B)	109.5
C(6)-C(7)-C(2)	121.77(17)	H(40A)-C(40)-H(40B)	109.5
C(6)-C(7)-N(2)	130.65(17)	C(37)-C(40)-H(40C)	109.5
C(2)-C(7)-N(2)	107.14(15)	H(40A)-C(40)-H(40C)	109.5
C(7)-N(2)-C(36)	123.81(15)	H(40B)-C(40)-H(40C)	109.5
C(7)-N(2)-C(1)	108.59(14)	C(34)-C(33)-C(32)	124.00(18)
C(36)-N(2)-C(1)	117.04(14)	C(34)-C(33)-H(33)	118.0
C(7)-N(2)-Zr(1)	118.27(11)	C(32)-C(33)-H(33)	118.0
C(36)-N(2)-Zr(1)	111.41(11)	C(35)-C(34)-C(33)	117.17(17)
C(1)-N(2)-Zr(1)	61.88(8)	C(35)-C(34)-C(41)	119.51(17)
C(31)-O(2)-Zr(1)	125.55(11)	C(33)-C(34)-C(41)	123.28(17)
O(2)-C(31)-C(36)	117.27(16)	C(36)-C(35)-C(34)	120.19(17)
O(2)-C(31)-C(32)	124.46(16)	C(36)-C(35)-H(35)	119.9
C(36)-C(31)-C(32)	118.27(17)	C(34)-C(35)-H(35)	119.9
C(33)-C(32)-C(31)	117.67(17)	C(43)-C(41)-C(42)	109.31(17)
C(33)-C(32)-C(37)	121.04(17)	C(43)-C(41)-C(34)	112.53(16)
C(31)-C(32)-C(37)	121.28(17)	C(42)-C(41)-C(34)	108.78(16)
C(40)-C(37)-C(38)	107.74(17)	C(43)-C(41)-C(44)	107.89(16)
C(40)-C(37)-C(32)	110.08(16)	C(42)-C(41)-C(44)	108.35(17)
C(38)-C(37)-C(32)	112.39(16)	C(34)-C(41)-C(44)	109.89(16)
C(40)-C(37)-C(39)	110.38(17)	C(41)-C(42)-H(42A)	109.5
C(38)-C(37)-C(39)	107.51(17)	C(41)-C(42)-H(42B)	109.5
C(32)-C(37)-C(39)	108.71(15)	H(42A)-C(42)-H(42B)	109.5

C(41)-C(42)-H(42C)	109.5	Zr(1)-C(61)-H(61B)	110.4
H(42A)-C(42)-H(42C)	109.5	H(61A)-C(61)-H(61B)	108.6
H(42B)-C(42)-H(42C)	109.5	C(67)-C(62)-C(63)	116.20(19)
C(41)-C(43)-H(43A)	109.5	C(67)-C(62)-C(61)	124.2(2)
C(41)-C(43)-H(43B)	109.5	C(63)-C(62)-C(61)	119.61(18)
H(43A)-C(43)-H(43B)	109.5	C(64)-C(63)-C(62)	122.1(2)
C(41)-C(43)-H(43C)	109.5	C(64)-C(63)-H(63)	119.0
H(43A)-C(43)-H(43C)	109.5	C(62)-C(63)-H(63)	119.0
H(43B)-C(43)-H(43C)	109.5	C(65)-C(64)-C(63)	119.7(2)
C(41)-C(44)-H(44A)	109.5	C(65)-C(64)-H(64)	120.2
C(41)-C(44)-H(44B)	109.5	C(63)-C(64)-H(64)	120.2
H(44A)-C(44)-H(44B)	109.5	C(66)-C(65)-C(64)	120.4(2)
C(41)-C(44)-H(44C)	109.5	C(66)-C(65)-H(65)	119.8
H(44A)-C(44)-H(44C)	109.5	C(64)-C(65)-H(65)	119.8
H(44B)-C(44)-H(44C)	109.5	C(65)-C(66)-C(67)	119.7(2)
C(35)-C(36)-C(31)	122.67(17)	C(65)-C(66)-H(66)	120.1
C(35)-C(36)-N(2)	122.77(16)	C(67)-C(66)-H(66)	120.1
C(31)-C(36)-N(2)	114.51(16)	C(62)-C(67)-C(66)	121.8(2)
C(62)-C(61)-Zr(1)	106.47(12)	C(62)-C(67)-H(67)	119.1
C(62)-C(61)-H(61A)	110.4	C(66)-C(67)-H(67)	119.1
Zr(1)-C(61)-H(61A)	110.4		
C(62)-C(61)-H(61B)	110.4		

b) Complex 3 (CCDC 1404597):

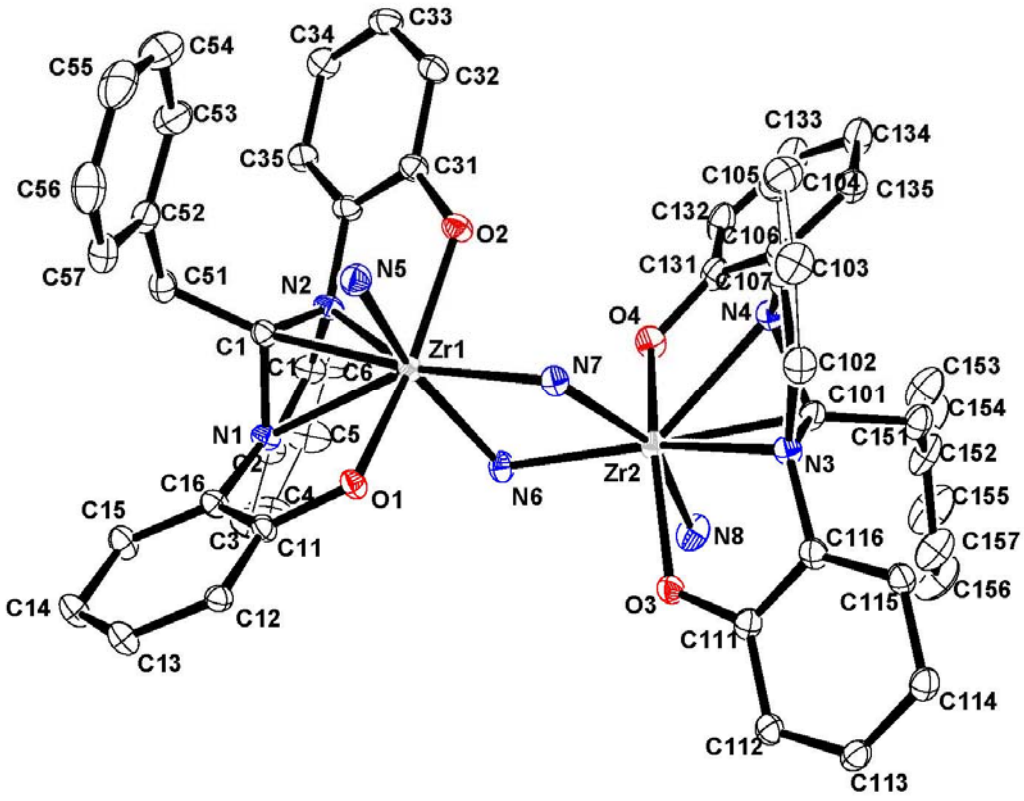

Figure S19: Molecular structure of complex **3**. For clarity, *tertio*-butyl and hydrogen atoms were omitted.

Table 3. Crystal data and structure refinement for complex **3**.

Empirical formula	C97.97 H145.53 N8 O4 Zr2	
Formula weight	1681.82	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 24.6453(7) Å	α= 90°.
	b = 19.6437(5) Å	β= 90.3251(17)°.
	c = 19.8192(6) Å	γ = 90°.
Volume	9594.8(5) $Å^3$	
Z	4	
Density (calculated)	1.164 Mg/m^3	

Absorption coefficient	2.172 mm^{-1}
F(000)	3605
Crystal size	0.200 x 0.100 x 0.050 mm^3
Theta range for data collection	2.877 to 74.913°.
Index ranges	-30<=h<=30, -24<=k<=24, -24<=l<=22
Reflections collected	177942
Independent reflections	19668 [R(int) = 0.1244]
Completeness to theta = 67.679°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7538 and 0.6800
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19668 / 897 / 1232
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.1551
R indices (all data)	R1 = 0.0915, wR2 = 0.1704
Extinction coefficient	n/a
Largest diff. peak and hole	1.282 and -0.752 e.$Å^{-3}$

Experimental details:

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Cu K_α radiation (λ = 1.54178 Å) from an IμS micro-source for the structure of compound **3**. The structure was solved by direct methods using SHELXS[3] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[4] using established refinement techniques.[5] All non-hydrogen atoms were refined anisotropically. Unless otherwise noted, all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3-distances. and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Compound **3** crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit along with 2.80 molecules of pentane. Two of the tert-butyl groups were disordered over two

positions and refined with the help of enhanced rigid bond restraints for the anisotropic displacement parameters. One of the benzyl groups was disordered over two positions and refined with the help of similarity restraints on the displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. The structure contains 1.80 molecules of pentane disordered over three unique positions which were refined with the help of similarity restraints on the displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. The elongated thermal ellipsoids on the pentane atoms and residual electron density around the pentane disorder suggest additional disorder could be modeled, however, the refinement of additional pentane positions did not improve the model. The coordinates for the hydrogen atoms bound to N5, N6, N7, and N8 were located in the difference Fourier synthesis and refined semi-freely with the help of a restraint on the N-H distance (0.91(4) Å).

Table 4. Bond lengths [Å] and angles [°] for complex **3**.

N(5)-Zr(1)	2.402(4)	C(55)-C(56)	1.378(9)
N(5)-H(5N1)	0.90(2)	C(55)-H(55)	0.9500
N(5)-H(5N3)	0.92(2)	C(56)-C(57)	1.384(8)
N(5)-H(5N2)	0.90(2)	C(56)-H(56)	0.9500
N(6)-Zr(1)	2.260(4)	C(57)-H(57)	0.9500
N(6)-Zr(2)	2.304(4)	N(1)-C(2)	1.427(5)
N(6)-H(6N1)	0.902(19)	N(1)-C(16)	1.432(5)
N(6)-H(6N2)	0.913(19)	O(1)-C(11)	1.339(5)
N(7)-Zr(2)	2.248(4)	C(11)-C(16)	1.402(6)
N(7)-Zr(1)	2.298(4)	C(11)-C(12)	1.408(6)
N(7)-H(7N1)	0.902(19)	C(12)-C(13)	1.405(6)
N(7)-H(7N2)	0.909(19)	C(12)-C(17)	1.533(6)
N(8)-Zr(2)	2.416(4)	C(17)-C(19)	1.525(6)
N(8)-H(8N1)	0.91(2)	C(17)-C(18)	1.538(6)
N(8)-H(8N2)	0.90(2)	C(17)-C(20)	1.539(6)
N(8)-H(8N3)	0.89(2)	C(18)-H(18A)	0.9800
Zr(1)-O(2)	2.072(3)	C(18)-H(18B)	0.9800
Zr(1)-O(1)	2.075(3)	C(18)-H(18C)	0.9800
Zr(1)-C(1)	2.214(4)	C(19)-H(19A)	0.9800
Zr(1)-N(2)	2.423(3)	C(19)-H(19B)	0.9800
Zr(1)-N(1)	2.474(3)	C(19)-H(19C)	0.9800
Zr(1)-Zr(2)	3.5177(5)	C(20)-H(20A)	0.9800
C(1)-N(1)	1.484(5)	C(20)-H(20B)	0.9800
C(1)-N(2)	1.502(5)	C(20)-H(20C)	0.9800
C(1)-C(51)	1.539(6)	C(13)-C(14)	1.393(6)
C(51)-C(52)	1.512(6)	C(13)-H(13)	0.9500
C(51)-H(51A)	0.9900	C(14)-C(15)	1.397(6)
C(51)-H(51B)	0.9900	C(14)-C(21)	1.538(6)
C(52)-C(53)	1.380(7)	C(21)-C(23)	1.496(8)
C(52)-C(57)	1.397(7)	C(21)-C(22)	1.501(7)
C(53)-C(54)	1.397(8)	C(21)-C(24)	1.581(9)
C(53)-H(53)	0.9500	C(22)-H(22A)	0.9800
C(54)-C(55)	1.386(9)	C(22)-H(22B)	0.9800
C(54)-H(54)	0.9500	C(22)-H(22C)	0.9800

C(23)-H(23A)	0.9800	C(40)-H(40C)	0.9800
C(23)-H(23B)	0.9800	C(33)-C(34)	1.385(7)
C(23)-H(23C)	0.9800	C(33)-H(33)	0.9500
C(24)-H(24A)	0.9800	C(34)-C(35)	1.399(6)
C(24)-H(24B)	0.9800	C(34)-C(41)	1.543(6)
C(24)-H(24C)	0.9800	C(41)-C(42A)	1.515(12)
C(15)-C(16)	1.390(6)	C(41)-C(43)	1.517(7)
C(15)-H(15)	0.9500	C(41)-C(44)	1.522(8)
C(2)-C(3)	1.374(6)	C(41)-C(43A)	1.522(12)
C(2)-C(7)	1.393(6)	C(41)-C(44A)	1.529(12)
C(3)-C(4)	1.403(7)	C(41)-C(42)	1.542(8)
C(3)-H(3)	0.9500	C(42)-H(42A)	0.9800
C(4)-C(5)	1.374(8)	C(42)-H(42B)	0.9800
C(4)-H(4)	0.9500	C(42)-H(42C)	0.9800
C(5)-C(6)	1.398(7)	C(43)-H(43A)	0.9800
C(5)-H(5)	0.9500	C(43)-H(43B)	0.9800
C(6)-C(7)	1.382(6)	C(43)-H(43C)	0.9800
C(6)-H(6)	0.9500	C(44)-H(44A)	0.9800
C(7)-N(2)	1.424(5)	C(44)-H(44B)	0.9800
N(2)-C(36)	1.443(5)	C(44)-H(44C)	0.9800
O(2)-C(31)	1.356(5)	C(42A)-H(42D)	0.9800
C(31)-C(36)	1.399(6)	C(42A)-H(42E)	0.9800
C(31)-C(32)	1.405(6)	C(42A)-H(42F)	0.9800
C(32)-C(33)	1.399(7)	C(43A)-H(43D)	0.9800
C(32)-C(37)	1.538(7)	C(43A)-H(43E)	0.9800
C(37)-C(39)	1.522(7)	C(43A)-H(43F)	0.9800
C(37)-C(40)	1.534(7)	C(44A)-H(44D)	0.9800
C(37)-C(38)	1.538(7)	C(44A)-H(44E)	0.9800
C(38)-H(38A)	0.9800	C(44A)-H(44F)	0.9800
C(38)-H(38B)	0.9800	C(35)-C(36)	1.383(6)
C(38)-H(38C)	0.9800	C(35)-H(35)	0.9500
C(39)-H(39A)	0.9800	Zr(2)-O(4)	2.094(3)
C(39)-H(39B)	0.9800	Zr(2)-O(3)	2.098(3)
C(39)-H(39C)	0.9800	Zr(2)-C(101)	2.218(4)
C(40)-H(40A)	0.9800	Zr(2)-N(4)	2.429(4)
C(40)-H(40B)	0.9800	Zr(2)-N(3)	2.461(3)

C(101)-N(4)	1.494(5)	C(112)-C(113)	1.398(6)
C(101)-N(3)	1.494(5)	C(112)-C(117)	1.535(6)
C(101)-C(151)	1.521(6)	C(117)-C(119)	1.530(6)
C(151)-C(152)	1.492(10)	C(117)-C(118)	1.532(7)
C(151)-C(52B)	1.521(12)	C(117)-C(120)	1.544(6)
C(151)-H(51C)	0.9900	C(118)-H(11A)	0.9800
C(151)-H(51D)	0.9900	C(118)-H(11B)	0.9800
C(151)-H(51E)	0.9900	C(118)-H(11C)	0.9800
C(151)-H(51F)	0.9900	C(119)-H(11D)	0.9800
C(152)-C(157)	1.383(11)	C(119)-H(11E)	0.9800
C(152)-C(153)	1.396(11)	C(119)-H(11F)	0.9800
C(153)-C(154)	1.378(12)	C(120)-H(12A)	0.9800
C(153)-H(153)	0.9500	C(120)-H(12B)	0.9800
C(154)-C(155)	1.398(13)	C(120)-H(12C)	0.9800
C(154)-H(154)	0.9500	C(113)-C(114)	1.394(7)
C(155)-C(156)	1.408(12)	C(113)-H(113)	0.9500
C(155)-H(155)	0.9500	C(114)-C(115)	1.390(6)
C(156)-C(157)	1.383(12)	C(114)-C(121)	1.542(6)
C(156)-H(156)	0.9500	C(121)-C(122)	1.532(6)
C(157)-H(157)	0.9500	C(121)-C(123)	1.535(7)
C(52B)-C(57B)	1.394(13)	C(121)-C(124)	1.536(7)
C(52B)-C(53B)	1.405(12)	C(122)-H(12D)	0.9800
C(53B)-C(54B)	1.378(14)	C(122)-H(12E)	0.9800
C(53B)-H(53B)	0.9500	C(122)-H(12F)	0.9800
C(54B)-C(55B)	1.409(15)	C(123)-H(12G)	0.9800
C(54B)-H(54B)	0.9500	C(123)-H(12H)	0.9800
C(55B)-C(56B)	1.402(14)	C(123)-H(12I)	0.9800
C(55B)-H(55B)	0.9500	C(124)-H(12J)	0.9800
C(56B)-C(57B)	1.387(13)	C(124)-H(12K)	0.9800
C(56B)-H(56B)	0.9500	C(124)-H(12L)	0.9800
C(57B)-H(57B)	0.9500	C(115)-C(116)	1.389(6)
N(3)-C(102)	1.401(6)	C(115)-H(115)	0.9500
N(3)-C(116)	1.437(5)	C(102)-C(103)	1.385(6)
O(3)-C(111)	1.341(5)	C(102)-C(107)	1.401(6)
C(111)-C(116)	1.391(6)	C(103)-C(104)	1.402(7)
C(111)-C(112)	1.428(6)	C(103)-H(103)	0.9500

C(104)-C(105)	1.382(7)	C(143)-H(14G)	0.9800
C(104)-H(104)	0.9500	C(143)-H(14H)	0.9800
C(105)-C(106)	1.405(7)	C(143)-H(14I)	0.9800
C(105)-H(105)	0.9500	C(144)-H(14J)	0.9800
C(106)-C(107)	1.371(7)	C(144)-H(14K)	0.9800
C(106)-H(106)	0.9500	C(144)-H(14L)	0.9800
C(107)-N(4)	1.422(6)	C(41B)-C(42B)	1.507(13)
N(4)-C(136)	1.436(5)	C(41B)-C(44B)	1.520(13)
O(4)-C(131)	1.340(6)	C(41B)-C(43B)	1.532(13)
C(131)-C(136)	1.400(7)	C(42B)-H(42G)	0.9800
C(131)-C(132)	1.406(6)	C(42B)-H(42H)	0.9800
C(132)-C(133)	1.385(8)	C(42B)-H(42I)	0.9800
C(132)-C(137)	1.544(8)	C(43B)-H(43G)	0.9800
C(137)-C(139)	1.532(8)	C(43B)-H(43H)	0.9800
C(137)-C(140)	1.542(10)	C(43B)-H(43I)	0.9800
C(137)-C(138)	1.543(8)	C(44B)-H(44G)	0.9800
C(138)-H(13A)	0.9800	C(44B)-H(44H)	0.9800
C(138)-H(13B)	0.9800	C(44B)-H(44I)	0.9800
C(138)-H(13C)	0.9800	C(135)-C(136)	1.378(7)
C(139)-H(13D)	0.9800	C(135)-H(135)	0.9500
C(139)-H(13E)	0.9800	C(11S)-C(12S)	1.499(10)
C(139)-H(13F)	0.9800	C(11S)-H(11G)	0.9800
C(140)-H(14A)	0.9800	C(11S)-H(11H)	0.9800
C(140)-H(14B)	0.9800	C(11S)-H(11I)	0.9800
C(140)-H(14C)	0.9800	C(12S)-C(13S)	1.469(10)
C(133)-C(134)	1.397(8)	C(12S)-H(12M)	0.9900
C(133)-H(133)	0.9500	C(12S)-H(12N)	0.9900
C(134)-C(135)	1.398(6)	C(13S)-C(14S)	1.488(10)
C(134)-C(41B)	1.527(13)	C(13S)-H(13G)	0.9900
C(134)-C(141)	1.551(10)	C(13S)-H(13H)	0.9900
C(141)-C(143)	1.524(11)	C(14S)-C(15S)	1.468(10)
C(141)-C(144)	1.536(12)	C(14S)-H(14M)	0.9900
C(141)-C(142)	1.540(11)	C(14S)-H(14N)	0.9900
C(142)-H(14D)	0.9800	C(15S)-H(15A)	0.9800
C(142)-H(14E)	0.9800	C(15S)-H(15B)	0.9800
C(142)-H(14F)	0.9800	C(15S)-H(15C)	0.9800

C(21S)-C(22S)	1.445(13)	C(42S)-C(43S)	1.454(14)
C(21S)-H(21A)	0.9800	C(42S)-H(42J)	0.9900
C(21S)-H(21B)	0.9800	C(42S)-H(42K)	0.9900
C(21S)-H(21C)	0.9800	C(43S)-C(44S)	1.469(15)
C(22S)-C(23S)	1.435(13)	C(43S)-H(43J)	0.9900
C(22S)-H(22D)	0.9900	C(43S)-H(43K)	0.9900
C(22S)-H(22E)	0.9900	C(44S)-C(45S)	1.444(15)
C(23S)-C(24S)	1.445(14)	C(44S)-H(44J)	0.9900
C(23S)-H(23D)	0.9900	C(44S)-H(44K)	0.9900
C(23S)-H(23E)	0.9900	C(45S)-H(45A)	0.9800
C(24S)-C(25S)	1.422(13)	C(45S)-H(45B)	0.9800
C(24S)-H(24D)	0.9900	C(45S)-H(45C)	0.9800
C(24S)-H(24E)	0.9900		
C(25S)-H(25A)	0.9800	Zr(1)-N(5)-H(5N1)	114(4)
C(25S)-H(25B)	0.9800	Zr(1)-N(5)-H(5N3)	111(4)
C(25S)-H(25C)	0.9800	H(5N1)-N(5)-H(5N3)	103(5)
C(31S)-C(32S)	1.443(10)	Zr(1)-N(5)-H(5N2)	106(4)
C(31S)-H(31A)	0.9800	H(5N1)-N(5)-H(5N2)	121(5)
C(31S)-H(31B)	0.9800	H(5N3)-N(5)-H(5N2)	99(5)
C(31S)-H(31C)	0.9800	Zr(1)-N(6)-Zr(2)	100.85(14)
C(32S)-C(33S)	1.396(8)	Zr(1)-N(6)-H(6N1)	109(3)
C(32S)-H(32A)	0.9900	Zr(2)-N(6)-H(6N1)	118(3)
C(32S)-H(32B)	0.9900	Zr(1)-N(6)-H(6N2)	111(3)
C(33S)-C(34S)	1.432(9)	Zr(2)-N(6)-H(6N2)	110(3)
C(33S)-H(33A)	0.9900	H(6N1)-N(6)-H(6N2)	108(5)
C(33S)-H(33B)	0.9900	Zr(2)-N(7)-Zr(1)	101.39(14)
C(34S)-C(35S)	1.399(10)	Zr(2)-N(7)-H(7N1)	118(3)
C(34S)-H(34A)	0.9900	Zr(1)-N(7)-H(7N1)	112(3)
C(34S)-H(34B)	0.9900	Zr(2)-N(7)-H(7N2)	111(3)
C(35S)-H(35A)	0.9800	Zr(1)-N(7)-H(7N2)	111(3)
C(35S)-H(35B)	0.9800	H(7N1)-N(7)-H(7N2)	104(4)
C(35S)-H(35C)	0.9800	Zr(2)-N(8)-H(8N1)	116(4)
C(41S)-C(42S)	1.413(15)	Zr(2)-N(8)-H(8N2)	117(4)
C(41S)-H(41A)	0.9800	H(8N1)-N(8)-H(8N2)	95(5)
C(41S)-H(41B)	0.9800	Zr(2)-N(8)-H(8N3)	114(4)
C(41S)-H(41C)	0.9800	H(8N1)-N(8)-H(8N3)	111(6)

H(8N2)-N(8)-H(8N3)	101(6)	N(1)-Zr(1)-Zr(2)	128.15(8)
O(2)-Zr(1)-O(1)	155.96(12)	N(1)-C(1)-N(2)	95.4(3)
O(2)-Zr(1)-C(1)	91.05(13)	N(1)-C(1)-C(51)	115.8(3)
O(1)-Zr(1)-C(1)	91.87(13)	N(2)-C(1)-C(51)	116.5(3)
O(2)-Zr(1)-N(6)	106.95(13)	N(1)-C(1)-Zr(1)	81.4(2)
O(1)-Zr(1)-N(6)	92.88(13)	N(2)-C(1)-Zr(1)	78.8(2)
C(1)-Zr(1)-N(6)	117.01(14)	C(51)-C(1)-Zr(1)	153.9(3)
O(2)-Zr(1)-N(7)	84.64(13)	C(52)-C(51)-C(1)	112.5(4)
O(1)-Zr(1)-N(7)	86.85(12)	C(52)-C(51)-H(51A)	109.1
C(1)-Zr(1)-N(7)	166.07(14)	C(1)-C(51)-H(51A)	109.1
N(6)-Zr(1)-N(7)	76.91(13)	C(52)-C(51)-H(51B)	109.1
O(2)-Zr(1)-N(5)	78.39(13)	C(1)-C(51)-H(51B)	109.1
O(1)-Zr(1)-N(5)	78.06(13)	H(51A)-C(51)-H(51B)	107.8
C(1)-Zr(1)-N(5)	85.52(14)	C(53)-C(52)-C(57)	118.7(5)
N(6)-Zr(1)-N(5)	156.23(13)	C(53)-C(52)-C(51)	121.7(4)
N(7)-Zr(1)-N(5)	80.65(13)	C(57)-C(52)-C(51)	119.5(4)
O(2)-Zr(1)-N(2)	70.59(12)	C(52)-C(53)-C(54)	121.2(5)
O(1)-Zr(1)-N(2)	123.02(11)	C(52)-C(53)-H(53)	119.4
C(1)-Zr(1)-N(2)	37.45(13)	C(54)-C(53)-H(53)	119.4
N(6)-Zr(1)-N(2)	92.62(13)	C(55)-C(54)-C(53)	119.3(6)
N(7)-Zr(1)-N(2)	149.14(12)	C(55)-C(54)-H(54)	120.4
N(5)-Zr(1)-N(2)	110.80(13)	C(53)-C(54)-H(54)	120.4
O(2)-Zr(1)-N(1)	122.73(11)	C(56)-C(55)-C(54)	119.9(6)
O(1)-Zr(1)-N(1)	69.89(11)	C(56)-C(55)-H(55)	120.1
C(1)-Zr(1)-N(1)	36.37(13)	C(54)-C(55)-H(55)	120.1
N(6)-Zr(1)-N(1)	88.75(12)	C(55)-C(56)-C(57)	120.7(5)
N(7)-Zr(1)-N(1)	152.11(12)	C(55)-C(56)-H(56)	119.7
N(5)-Zr(1)-N(1)	108.12(13)	C(57)-C(56)-H(56)	119.7
N(2)-Zr(1)-N(1)	53.60(11)	C(56)-C(57)-C(52)	120.2(5)
O(2)-Zr(1)-Zr(2)	88.15(9)	C(56)-C(57)-H(57)	119.9
O(1)-Zr(1)-Zr(2)	99.12(8)	C(52)-C(57)-H(57)	119.9
C(1)-Zr(1)-Zr(2)	154.55(11)	C(2)-N(1)-C(16)	123.2(3)
N(6)-Zr(1)-Zr(2)	40.03(9)	C(2)-N(1)-C(1)	109.2(3)
N(7)-Zr(1)-Zr(2)	38.79(9)	C(16)-N(1)-C(1)	118.6(3)
N(5)-Zr(1)-Zr(2)	119.12(10)	C(2)-N(1)-Zr(1)	118.8(3)
N(2)-Zr(1)-Zr(2)	119.80(9)	C(16)-N(1)-Zr(1)	109.9(2)

C(1)-N(1)-Zr(1)	62.3(2)	C(13)-C(14)-C(21)	122.7(4)
C(11)-O(1)-Zr(1)	125.8(3)	C(15)-C(14)-C(21)	120.0(4)
O(1)-C(11)-C(16)	117.8(4)	C(23)-C(21)-C(22)	113.6(5)
O(1)-C(11)-C(12)	123.1(4)	C(23)-C(21)-C(14)	110.1(4)
C(16)-C(11)-C(12)	119.1(4)	C(22)-C(21)-C(14)	113.4(4)
C(13)-C(12)-C(11)	117.2(4)	C(23)-C(21)-C(24)	106.1(5)
C(13)-C(12)-C(17)	122.2(4)	C(22)-C(21)-C(24)	104.8(5)
C(11)-C(12)-C(17)	120.6(4)	C(14)-C(21)-C(24)	108.4(4)
C(19)-C(17)-C(12)	112.6(3)	C(21)-C(22)-H(22A)	109.5
C(19)-C(17)-C(18)	108.4(4)	C(21)-C(22)-H(22B)	109.5
C(12)-C(17)-C(18)	109.6(3)	H(22A)-C(22)-H(22B)	109.5
C(19)-C(17)-C(20)	106.7(3)	C(21)-C(22)-H(22C)	109.5
C(12)-C(17)-C(20)	109.1(3)	H(22A)-C(22)-H(22C)	109.5
C(18)-C(17)-C(20)	110.4(4)	H(22B)-C(22)-H(22C)	109.5
C(17)-C(18)-H(18A)	109.5	C(21)-C(23)-H(23A)	109.5
C(17)-C(18)-H(18B)	109.5	C(21)-C(23)-H(23B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(17)-C(18)-H(18C)	109.5	C(21)-C(23)-H(23C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(18B)-C(18)-H(18C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(17)-C(19)-H(19A)	109.5	C(21)-C(24)-H(24A)	109.5
C(17)-C(19)-H(19B)	109.5	C(21)-C(24)-H(24B)	109.5
H(19A)-C(19)-H(19B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(17)-C(19)-H(19C)	109.5	C(21)-C(24)-H(24C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(19B)-C(19)-H(19C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(17)-C(20)-H(20A)	109.5	C(16)-C(15)-C(14)	120.0(4)
C(17)-C(20)-H(20B)	109.5	C(16)-C(15)-H(15)	120.0
H(20A)-C(20)-H(20B)	109.5	C(14)-C(15)-H(15)	120.0
C(17)-C(20)-H(20C)	109.5	C(15)-C(16)-C(11)	122.1(4)
H(20A)-C(20)-H(20C)	109.5	C(15)-C(16)-N(1)	123.2(4)
H(20B)-C(20)-H(20C)	109.5	C(11)-C(16)-N(1)	114.7(4)
C(14)-C(13)-C(12)	124.2(4)	C(3)-C(2)-C(7)	122.0(4)
C(14)-C(13)-H(13)	117.9	C(3)-C(2)-N(1)	131.8(4)
C(12)-C(13)-H(13)	117.9	C(7)-C(2)-N(1)	105.9(4)
C(13)-C(14)-C(15)	117.3(4)	C(2)-C(3)-C(4)	117.4(5)

C(2)-C(3)-H(3)	121.3	C(37)-C(38)-H(38C)	109.5
C(4)-C(3)-H(3)	121.3	H(38A)-C(38)-H(38C)	109.5
C(5)-C(4)-C(3)	120.6(5)	H(38B)-C(38)-H(38C)	109.5
C(5)-C(4)-H(4)	119.7	C(37)-C(39)-H(39A)	109.5
C(3)-C(4)-H(4)	119.7	C(37)-C(39)-H(39B)	109.5
C(4)-C(5)-C(6)	121.9(5)	H(39A)-C(39)-H(39B)	109.5
C(4)-C(5)-H(5)	119.0	C(37)-C(39)-H(39C)	109.5
C(6)-C(5)-H(5)	119.0	H(39A)-C(39)-H(39C)	109.5
C(7)-C(6)-C(5)	117.3(5)	H(39B)-C(39)-H(39C)	109.5
C(7)-C(6)-H(6)	121.3	C(37)-C(40)-H(40A)	109.5
C(5)-C(6)-H(6)	121.3	C(37)-C(40)-H(40B)	109.5
C(6)-C(7)-C(2)	120.7(4)	H(40A)-C(40)-H(40B)	109.5
C(6)-C(7)-N(2)	131.8(4)	C(37)-C(40)-H(40C)	109.5
C(2)-C(7)-N(2)	107.3(4)	H(40A)-C(40)-H(40C)	109.5
C(7)-N(2)-C(36)	123.3(3)	H(40B)-C(40)-H(40C)	109.5
C(7)-N(2)-C(1)	108.2(3)	C(34)-C(33)-C(32)	124.7(4)
C(36)-N(2)-C(1)	116.5(3)	C(34)-C(33)-H(33)	117.7
C(7)-N(2)-Zr(1)	119.3(3)	C(32)-C(33)-H(33)	117.7
C(36)-N(2)-Zr(1)	111.0(3)	C(33)-C(34)-C(35)	117.8(4)
C(1)-N(2)-Zr(1)	63.71(19)	C(33)-C(34)-C(41)	122.9(4)
C(31)-O(2)-Zr(1)	125.2(3)	C(35)-C(34)-C(41)	119.2(4)
O(2)-C(31)-C(36)	116.8(4)	C(43)-C(41)-C(44)	110.1(5)
O(2)-C(31)-C(32)	123.7(4)	C(42A)-C(41)-C(43A)	110.0(9)
C(36)-C(31)-C(32)	119.5(4)	C(42A)-C(41)-C(44A)	112.0(9)
C(33)-C(32)-C(31)	116.4(4)	C(43A)-C(41)-C(44A)	107.1(9)
C(33)-C(32)-C(37)	122.3(4)	C(43)-C(41)-C(42)	106.7(5)
C(31)-C(32)-C(37)	121.3(4)	C(44)-C(41)-C(42)	108.6(5)
C(39)-C(37)-C(40)	110.1(5)	C(42A)-C(41)-C(34)	106.1(10)
C(39)-C(37)-C(32)	109.8(4)	C(43)-C(41)-C(34)	112.9(5)
C(40)-C(37)-C(32)	109.4(4)	C(44)-C(41)-C(34)	109.5(4)
C(39)-C(37)-C(38)	108.3(4)	C(43A)-C(41)-C(34)	112.4(10)
C(40)-C(37)-C(38)	107.8(4)	C(44A)-C(41)-C(34)	109.2(11)
C(32)-C(37)-C(38)	111.3(4)	C(42)-C(41)-C(34)	109.0(4)
C(37)-C(38)-H(38A)	109.5	C(41)-C(42)-H(42A)	109.5
C(37)-C(38)-H(38B)	109.5	C(41)-C(42)-H(42B)	109.5
H(38A)-C(38)-H(38B)	109.5	H(42A)-C(42)-H(42B)	109.5

C(41)-C(42)-H(42C)	109.5	C(35)-C(36)-C(31)	122.6(4)
H(42A)-C(42)-H(42C)	109.5	C(35)-C(36)-N(2)	122.9(4)
H(42B)-C(42)-H(42C)	109.5	C(31)-C(36)-N(2)	114.5(4)
C(41)-C(43)-H(43A)	109.5	O(4)-Zr(2)-O(3)	154.31(12)
C(41)-C(43)-H(43B)	109.5	O(4)-Zr(2)-C(101)	89.85(14)
H(43A)-C(43)-H(43B)	109.5	O(3)-Zr(2)-C(101)	90.43(13)
C(41)-C(43)-H(43C)	109.5	O(4)-Zr(2)-N(7)	103.81(13)
H(43A)-C(43)-H(43C)	109.5	O(3)-Zr(2)-N(7)	99.68(12)
H(43B)-C(43)-H(43C)	109.5	C(101)-Zr(2)-N(7)	113.04(15)
C(41)-C(44)-H(44A)	109.5	O(4)-Zr(2)-N(6)	79.41(13)
C(41)-C(44)-H(44B)	109.5	O(3)-Zr(2)-N(6)	96.07(13)
H(44A)-C(44)-H(44B)	109.5	C(101)-Zr(2)-N(6)	166.98(14)
C(41)-C(44)-H(44C)	109.5	N(7)-Zr(2)-N(6)	77.03(13)
H(44A)-C(44)-H(44C)	109.5	O(4)-Zr(2)-N(8)	76.96(14)
H(44B)-C(44)-H(44C)	109.5	O(3)-Zr(2)-N(8)	77.36(14)
C(41)-C(42A)-H(42D)	109.5	C(101)-Zr(2)-N(8)	89.38(16)
C(41)-C(42A)-H(42E)	109.5	N(7)-Zr(2)-N(8)	157.50(15)
H(42D)-C(42A)-H(42E)	109.5	N(6)-Zr(2)-N(8)	81.09(14)
C(41)-C(42A)-H(42F)	109.5	O(4)-Zr(2)-N(4)	69.61(12)
H(42D)-C(42A)-H(42F)	109.5	O(3)-Zr(2)-N(4)	122.17(11)
H(42E)-C(42A)-H(42F)	109.5	C(101)-Zr(2)-N(4)	37.16(14)
C(41)-C(43A)-H(43D)	109.5	N(7)-Zr(2)-N(4)	87.38(13)
C(41)-C(43A)-H(43E)	109.5	N(6)-Zr(2)-N(4)	140.78(13)
H(43D)-C(43A)-H(43E)	109.5	N(8)-Zr(2)-N(4)	113.29(14)
C(41)-C(43A)-H(43F)	109.5	O(4)-Zr(2)-N(3)	121.78(12)
H(43D)-C(43A)-H(43F)	109.5	O(3)-Zr(2)-N(3)	69.59(11)
H(43E)-C(43A)-H(43F)	109.5	C(101)-Zr(2)-N(3)	36.79(13)
C(41)-C(44A)-H(44D)	109.5	N(7)-Zr(2)-N(3)	86.44(12)
C(41)-C(44A)-H(44E)	109.5	N(6)-Zr(2)-N(3)	156.12(12)
H(44D)-C(44A)-H(44E)	109.5	N(8)-Zr(2)-N(3)	112.61(13)
C(41)-C(44A)-H(44F)	109.5	N(4)-Zr(2)-N(3)	53.54(11)
H(44D)-C(44A)-H(44F)	109.5	O(4)-Zr(2)-Zr(1)	83.05(9)
H(44E)-C(44A)-H(44F)	109.5	O(3)-Zr(2)-Zr(1)	109.45(8)
C(36)-C(35)-C(34)	119.0(4)	C(101)-Zr(2)-Zr(1)	147.26(11)
C(36)-C(35)-H(35)	120.5	N(7)-Zr(2)-Zr(1)	39.82(9)
C(34)-C(35)-H(35)	120.5	N(6)-Zr(2)-Zr(1)	39.12(9)

N(8)-Zr(2)-Zr(1)	119.62(11)	C(156)-C(157)-C(152)	121.0(10)
N(4)-Zr(2)-Zr(1)	111.54(9)	C(156)-C(157)-H(157)	119.5
N(3)-Zr(2)-Zr(1)	126.22(8)	C(152)-C(157)-H(157)	119.5
N(4)-C(101)-N(3)	95.0(3)	C(57B)-C(52B)-C(53B)	116.9(13)
N(4)-C(101)-C(151)	116.7(4)	C(57B)-C(52B)-C(151)	118.6(12)
N(3)-C(101)-C(151)	117.0(3)	C(53B)-C(52B)-C(151)	123.4(13)
N(4)-C(101)-Zr(2)	79.1(2)	C(54B)-C(53B)-C(52B)	122.5(13)
N(3)-C(101)-Zr(2)	80.5(2)	C(54B)-C(53B)-H(53B)	118.8
C(151)-C(101)-Zr(2)	153.3(3)	C(52B)-C(53B)-H(53B)	118.8
C(152)-C(151)-C(101)	112.6(11)	C(53B)-C(54B)-C(55B)	119.1(13)
C(52B)-C(151)-C(101)	110.1(14)	C(53B)-C(54B)-H(54B)	120.5
C(152)-C(151)-H(51C)	109.1	C(55B)-C(54B)-H(54B)	120.5
C(101)-C(151)-H(51C)	109.1	C(56B)-C(55B)-C(54B)	119.7(13)
C(152)-C(151)-H(51D)	109.1	C(56B)-C(55B)-H(55B)	120.1
C(101)-C(151)-H(51D)	109.1	C(54B)-C(55B)-H(55B)	120.1
H(51C)-C(151)-H(51D)	107.8	C(57B)-C(56B)-C(55B)	119.2(14)
C(52B)-C(151)-H(51E)	109.6	C(57B)-C(56B)-H(56B)	120.4
C(101)-C(151)-H(51E)	109.6	C(55B)-C(56B)-H(56B)	120.4
C(52B)-C(151)-H(51F)	109.6	C(56B)-C(57B)-C(52B)	122.5(13)
C(101)-C(151)-H(51F)	109.6	C(56B)-C(57B)-H(57B)	118.8
H(51E)-C(151)-H(51F)	108.1	C(52B)-C(57B)-H(57B)	118.8
C(157)-C(152)-C(153)	119.8(9)	C(102)-N(3)-C(116)	123.5(3)
C(157)-C(152)-C(151)	120.3(10)	C(102)-N(3)-C(101)	110.0(3)
C(153)-C(152)-C(151)	119.9(10)	C(116)-N(3)-C(101)	117.6(3)
C(154)-C(153)-C(152)	121.1(11)	C(102)-N(3)-Zr(2)	116.9(3)
C(154)-C(153)-H(153)	119.4	C(116)-N(3)-Zr(2)	111.1(3)
C(152)-C(153)-H(153)	119.4	C(101)-N(3)-Zr(2)	62.8(2)
C(153)-C(154)-C(155)	118.0(10)	C(111)-O(3)-Zr(2)	125.2(3)
C(153)-C(154)-H(154)	121.0	O(3)-C(111)-C(116)	118.4(4)
C(155)-C(154)-H(154)	121.0	O(3)-C(111)-C(112)	124.1(4)
C(154)-C(155)-C(156)	122.0(10)	C(116)-C(111)-C(112)	117.4(4)
C(154)-C(155)-H(155)	119.0	C(113)-C(112)-C(111)	117.0(4)
C(156)-C(155)-H(155)	119.0	C(113)-C(112)-C(117)	122.5(4)
C(157)-C(156)-C(155)	118.0(11)	C(111)-C(112)-C(117)	120.5(4)
C(157)-C(156)-H(156)	121.0	C(119)-C(117)-C(118)	108.6(4)
C(155)-C(156)-H(156)	121.0	C(119)-C(117)-C(112)	112.0(4)

C(118)-C(117)-C(112)	109.6(4)	H(12D)-C(122)-H(12E)	109.5
C(119)-C(117)-C(120)	107.5(4)	C(121)-C(122)-H(12F)	109.5
C(118)-C(117)-C(120)	109.8(4)	H(12D)-C(122)-H(12F)	109.5
C(112)-C(117)-C(120)	109.3(4)	H(12E)-C(122)-H(12F)	109.5
C(117)-C(118)-H(11A)	109.5	C(121)-C(123)-H(12G)	109.5
C(117)-C(118)-H(11B)	109.5	C(121)-C(123)-H(12H)	109.5
H(11A)-C(118)-H(11B)	109.5	H(12G)-C(123)-H(12H)	109.5
C(117)-C(118)-H(11C)	109.5	C(121)-C(123)-H(12I)	109.5
H(11A)-C(118)-H(11C)	109.5	H(12G)-C(123)-H(12I)	109.5
H(11B)-C(118)-H(11C)	109.5	H(12H)-C(123)-H(12I)	109.5
C(117)-C(119)-H(11D)	109.5	C(121)-C(124)-H(12J)	109.5
C(117)-C(119)-H(11E)	109.5	C(121)-C(124)-H(12K)	109.5
H(11D)-C(119)-H(11E)	109.5	H(12J)-C(124)-H(12K)	109.5
C(117)-C(119)-H(11F)	109.5	C(121)-C(124)-H(12L)	109.5
H(11D)-C(119)-H(11F)	109.5	H(12J)-C(124)-H(12L)	109.5
H(11E)-C(119)-H(11F)	109.5	H(12K)-C(124)-H(12L)	109.5
C(117)-C(120)-H(12A)	109.5	C(116)-C(115)-C(114)	119.0(4)
C(117)-C(120)-H(12B)	109.5	C(116)-C(115)-H(115)	120.5
H(12A)-C(120)-H(12B)	109.5	C(114)-C(115)-H(115)	120.5
C(117)-C(120)-H(12C)	109.5	C(115)-C(116)-C(111)	124.3(4)
H(12A)-C(120)-H(12C)	109.5	C(115)-C(116)-N(3)	121.6(4)
H(12B)-C(120)-H(12C)	109.5	C(111)-C(116)-N(3)	114.1(4)
C(114)-C(113)-C(112)	125.0(4)	C(103)-C(102)-N(3)	131.4(4)
C(114)-C(113)-H(113)	117.5	C(103)-C(102)-C(107)	121.0(4)
C(112)-C(113)-H(113)	117.5	N(3)-C(102)-C(107)	107.2(4)
C(115)-C(114)-C(113)	117.3(4)	C(102)-C(103)-C(104)	117.5(4)
C(115)-C(114)-C(121)	122.3(4)	C(102)-C(103)-H(103)	121.3
C(113)-C(114)-C(121)	120.4(4)	C(104)-C(103)-H(103)	121.3
C(122)-C(121)-C(123)	108.0(4)	C(105)-C(104)-C(103)	121.1(4)
C(122)-C(121)-C(124)	109.7(4)	C(105)-C(104)-H(104)	119.4
C(123)-C(121)-C(124)	107.9(4)	C(103)-C(104)-H(104)	119.4
C(122)-C(121)-C(114)	109.2(4)	C(104)-C(105)-C(106)	121.2(5)
C(123)-C(121)-C(114)	111.7(4)	C(104)-C(105)-H(105)	119.4
C(124)-C(121)-C(114)	110.3(4)	C(106)-C(105)-H(105)	119.4
C(121)-C(122)-H(12D)	109.5	C(107)-C(106)-C(105)	117.6(4)
C(121)-C(122)-H(12E)	109.5	C(107)-C(106)-H(106)	121.2

C(105)-C(106)-H(106)	121.2	C(137)-C(140)-H(14B)	109.5
C(106)-C(107)-C(102)	121.6(4)	H(14A)-C(140)-H(14B)	109.5
C(106)-C(107)-N(4)	132.2(4)	C(137)-C(140)-H(14C)	109.5
C(102)-C(107)-N(4)	105.8(4)	H(14A)-C(140)-H(14C)	109.5
C(107)-N(4)-C(136)	123.0(4)	H(14B)-C(140)-H(14C)	109.5
C(107)-N(4)-C(101)	109.8(3)	C(132)-C(133)-C(134)	124.6(4)
C(136)-N(4)-C(101)	116.0(3)	C(132)-C(133)-H(133)	117.7
C(107)-N(4)-Zr(2)	117.9(3)	C(134)-C(133)-H(133)	117.7
C(136)-N(4)-Zr(2)	111.9(3)	C(133)-C(134)-C(135)	117.3(5)
C(101)-N(4)-Zr(2)	63.7(2)	C(133)-C(134)-C(41B)	118.7(7)
C(131)-O(4)-Zr(2)	125.6(3)	C(135)-C(134)-C(41B)	123.3(7)
O(4)-C(131)-C(136)	117.3(4)	C(133)-C(134)-C(141)	123.3(6)
O(4)-C(131)-C(132)	124.5(4)	C(135)-C(134)-C(141)	119.4(6)
C(136)-C(131)-C(132)	118.2(4)	C(143)-C(141)-C(144)	108.9(10)
C(133)-C(132)-C(131)	117.5(5)	C(143)-C(141)-C(142)	106.6(9)
C(133)-C(132)-C(137)	121.5(5)	C(144)-C(141)-C(142)	106.9(9)
C(131)-C(132)-C(137)	121.0(5)	C(143)-C(141)-C(134)	112.1(8)
C(139)-C(137)-C(140)	109.3(6)	C(144)-C(141)-C(134)	107.5(9)
C(139)-C(137)-C(138)	107.8(5)	C(142)-C(141)-C(134)	114.6(7)
C(140)-C(137)-C(138)	109.6(6)	C(141)-C(142)-H(14D)	109.5
C(139)-C(137)-C(132)	109.2(5)	C(141)-C(142)-H(14E)	109.5
C(140)-C(137)-C(132)	109.9(5)	H(14D)-C(142)-H(14E)	109.5
C(138)-C(137)-C(132)	111.1(6)	C(141)-C(142)-H(14F)	109.5
C(137)-C(138)-H(13A)	109.5	H(14D)-C(142)-H(14F)	109.5
C(137)-C(138)-H(13B)	109.5	H(14E)-C(142)-H(14F)	109.5
H(13A)-C(138)-H(13B)	109.5	C(141)-C(143)-H(14G)	109.5
C(137)-C(138)-H(13C)	109.5	C(141)-C(143)-H(14H)	109.5
H(13A)-C(138)-H(13C)	109.5	H(14G)-C(143)-H(14H)	109.5
H(13B)-C(138)-H(13C)	109.5	C(141)-C(143)-H(14I)	109.5
C(137)-C(139)-H(13D)	109.5	H(14G)-C(143)-H(14I)	109.5
C(137)-C(139)-H(13E)	109.5	H(14H)-C(143)-H(14I)	109.5
H(13D)-C(139)-H(13E)	109.5	C(141)-C(144)-H(14J)	109.5
C(137)-C(139)-H(13F)	109.5	C(141)-C(144)-H(14K)	109.5
H(13D)-C(139)-H(13F)	109.5	H(14J)-C(144)-H(14K)	109.5
H(13E)-C(139)-H(13F)	109.5	C(141)-C(144)-H(14L)	109.5
C(137)-C(140)-H(14A)	109.5	H(14J)-C(144)-H(14L)	109.5

H(14K)-C(144)-H(14L)	109.5	H(11H)-C(11S)-H(11I)	109.5
C(42B)-C(41B)-C(44B)	110.0(12)	C(13S)-C(12S)-C(11S)	116.6(8)
C(42B)-C(41B)-C(134)	113.7(10)	C(13S)-C(12S)-H(12M)	108.1
C(44B)-C(41B)-C(134)	104.2(10)	C(11S)-C(12S)-H(12M)	108.1
C(42B)-C(41B)-C(43B)	109.3(11)	C(13S)-C(12S)-H(12N)	108.1
C(44B)-C(41B)-C(43B)	110.0(12)	C(11S)-C(12S)-H(12N)	108.1
C(134)-C(41B)-C(43B)	109.6(10)	H(12M)-C(12S)-H(12N)	107.3
C(41B)-C(42B)-H(42G)	109.5	C(12S)-C(13S)-C(14S)	116.6(8)
C(41B)-C(42B)-H(42H)	109.5	C(12S)-C(13S)-H(13G)	108.1
H(42G)-C(42B)-H(42H)	109.5	C(14S)-C(13S)-H(13G)	108.1
C(41B)-C(42B)-H(42I)	109.5	C(12S)-C(13S)-H(13H)	108.1
H(42G)-C(42B)-H(42I)	109.5	C(14S)-C(13S)-H(13H)	108.1
H(42H)-C(42B)-H(42I)	109.5	H(13G)-C(13S)-H(13H)	107.3
C(41B)-C(43B)-H(43G)	109.5	C(15S)-C(14S)-C(13S)	115.3(8)
C(41B)-C(43B)-H(43H)	109.5	C(15S)-C(14S)-H(14M)	108.4
H(43G)-C(43B)-H(43H)	109.5	C(13S)-C(14S)-H(14M)	108.4
C(41B)-C(43B)-H(43I)	109.5	C(15S)-C(14S)-H(14N)	108.4
H(43G)-C(43B)-H(43I)	109.5	C(13S)-C(14S)-H(14N)	108.4
H(43H)-C(43B)-H(43I)	109.5	H(14M)-C(14S)-H(14N)	107.5
C(41B)-C(44B)-H(44G)	109.5	C(14S)-C(15S)-H(15A)	109.5
C(41B)-C(44B)-H(44H)	109.5	C(14S)-C(15S)-H(15B)	109.5
H(44G)-C(44B)-H(44H)	109.5	H(15A)-C(15S)-H(15B)	109.5
C(41B)-C(44B)-H(44I)	109.5	C(14S)-C(15S)-H(15C)	109.5
H(44G)-C(44B)-H(44I)	109.5	H(15A)-C(15S)-H(15C)	109.5
H(44H)-C(44B)-H(44I)	109.5	H(15B)-C(15S)-H(15C)	109.5
C(136)-C(135)-C(134)	119.0(5)	C(22S)-C(21S)-H(21A)	109.5
C(136)-C(135)-H(135)	120.5	C(22S)-C(21S)-H(21B)	109.5
C(134)-C(135)-H(135)	120.5	H(21A)-C(21S)-H(21B)	109.5
C(135)-C(136)-C(131)	123.4(4)	C(22S)-C(21S)-H(21C)	109.5
C(135)-C(136)-N(4)	122.7(4)	H(21A)-C(21S)-H(21C)	109.5
C(131)-C(136)-N(4)	113.8(4)	H(21B)-C(21S)-H(21C)	109.5
C(12S)-C(11S)-H(11G)	109.5	C(23S)-C(22S)-C(21S)	123.4(15)
C(12S)-C(11S)-H(11H)	109.5	C(23S)-C(22S)-H(22D)	106.5
H(11G)-C(11S)-H(11H)	109.5	C(21S)-C(22S)-H(22D)	106.5
C(12S)-C(11S)-H(11I)	109.5	C(23S)-C(22S)-H(22E)	106.5
H(11G)-C(11S)-H(11I)	109.5	C(21S)-C(22S)-H(22E)	106.5

H(22D)-C(22S)-H(22E)	106.5	H(33A)-C(33S)-H(33B)	106.7
C(22S)-C(23S)-C(24S)	119.3(15)	C(35S)-C(34S)-C(33S)	125.0(10)
C(22S)-C(23S)-H(23D)	107.5	C(35S)-C(34S)-H(34A)	106.1
C(24S)-C(23S)-H(23D)	107.5	C(33S)-C(34S)-H(34A)	106.1
C(22S)-C(23S)-H(23E)	107.5	C(35S)-C(34S)-H(34B)	106.1
C(24S)-C(23S)-H(23E)	107.5	C(33S)-C(34S)-H(34B)	106.1
H(23D)-C(23S)-H(23E)	107.0	H(34A)-C(34S)-H(34B)	106.3
C(25S)-C(24S)-C(23S)	119.9(16)	C(34S)-C(35S)-H(35A)	109.5
C(25S)-C(24S)-H(24D)	107.3	C(34S)-C(35S)-H(35B)	109.5
C(23S)-C(24S)-H(24D)	107.3	H(35A)-C(35S)-H(35B)	109.5
C(25S)-C(24S)-H(24E)	107.3	C(34S)-C(35S)-H(35C)	109.5
C(23S)-C(24S)-H(24E)	107.3	H(35A)-C(35S)-H(35C)	109.5
H(24D)-C(24S)-H(24E)	106.9	H(35B)-C(35S)-H(35C)	109.5
C(24S)-C(25S)-H(25A)	109.5	C(42S)-C(41S)-H(41A)	109.5
C(24S)-C(25S)-H(25B)	109.5	C(42S)-C(41S)-H(41B)	109.5
H(25A)-C(25S)-H(25B)	109.5	H(41A)-C(41S)-H(41B)	109.5
C(24S)-C(25S)-H(25C)	109.5	C(42S)-C(41S)-H(41C)	109.5
H(25A)-C(25S)-H(25C)	109.5	H(41A)-C(41S)-H(41C)	109.5
H(25B)-C(25S)-H(25C)	109.5	H(41B)-C(41S)-H(41C)	109.5
C(32S)-C(31S)-H(31A)	109.5	C(41S)-C(42S)-C(43S)	120.5(17)
C(32S)-C(31S)-H(31B)	109.5	C(41S)-C(42S)-H(42J)	107.2
H(31A)-C(31S)-H(31B)	109.5	C(43S)-C(42S)-H(42J)	107.2
C(32S)-C(31S)-H(31C)	109.5	C(41S)-C(42S)-H(42K)	107.2
H(31A)-C(31S)-H(31C)	109.5	C(43S)-C(42S)-H(42K)	107.2
H(31B)-C(31S)-H(31C)	109.5	H(42J)-C(42S)-H(42K)	106.8
C(33S)-C(32S)-C(31S)	120.5(8)	C(42S)-C(43S)-C(44S)	118.8(17)
C(33S)-C(32S)-H(32A)	107.2	C(42S)-C(43S)-H(43J)	107.6
C(31S)-C(32S)-H(32A)	107.2	C(44S)-C(43S)-H(43J)	107.6
C(33S)-C(32S)-H(32B)	107.2	C(42S)-C(43S)-H(43K)	107.6
C(31S)-C(32S)-H(32B)	107.2	C(44S)-C(43S)-H(43K)	107.6
H(32A)-C(32S)-H(32B)	106.8	H(43J)-C(43S)-H(43K)	107.1
C(32S)-C(33S)-C(34S)	121.7(7)	C(45S)-C(44S)-C(43S)	118.3(18)
C(32S)-C(33S)-H(33A)	106.9	C(45S)-C(44S)-H(44J)	107.7
C(34S)-C(33S)-H(33A)	106.9	C(43S)-C(44S)-H(44J)	107.7
C(32S)-C(33S)-H(33B)	106.9	C(45S)-C(44S)-H(44K)	107.7
C(34S)-C(33S)-H(33B)	106.9	C(43S)-C(44S)-H(44K)	107.7

H(44J)-C(44S)-H(44K)	107.1	C(44S)-C(45S)-H(45C)	109.5
C(44S)-C(45S)-H(45A)	109.5	H(45A)-C(45S)-H(45C)	109.5
C(44S)-C(45S)-H(45B)	109.5	H(45B)-C(45S)-H(45C)	109.5
H(45A)-C(45S)-H(45B)	109.5		

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